09/926,491 Page 1

=> d ibib ab hitstr 1-3

AA

Z

RX (9) RCT R 97452-84-1, Q 97452-83-0

STAGE(1)

RGT U 7601-90-3 HClO4 SOL 7732-18-5 Water, 67-56-1 MeOH

STAGE(2)

RGT V 1333-74-0 H2 CAT 1314-15-4 PtO2

PRO Z 97452-85-2, AA 97452-86-3

09/926,491 Page 1

L3 ANSWER 4 OF 4 CASREACT COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 103:71583 CASREACT

TITLE: A stereoselective synthesis of 1,2-diols from

.alpha.-hydroxyaldehydes

AUTHOR(S): Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.;

Russell, Graeme B.; Horn, Dennis H. S.

CORPORATE SOURCE: Dep. Chem., Univ. Wyoming, Laramie, WY, 82071, USA

SOURCE: Tetrahedron Letters (1985), 26(9), 1189-92

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal LANGUAGE: English

AB The addn. of LiC.tplbond.CCMe2O-THP (THP = tetrahydro-2H-pyran-2-yl) to (20R)-20-hydroxypregnane-20-carboxaldehydes I and II in the absence and in

the presence of BF3 afforded predominantly 20R,22R-diols III and IV or

20R,22S-diols V and VI, resp., characteristic of ecdysones.

RX(9) OF 53 ... **R** + Q ===> **Z** + AA

R

Q

09/926,491

=> s l1 and 19850804/ed 11811 19850804/ED (850804/ED) L11 1 L1 AND 19850804/ED

=> d

L11 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS on STN

RN 97452-85-2 REGISTRY

CN 19-Norcholesta-1,3,5(10)-triene-22,25-diol, 3-methoxy-, (22R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C27 H42 O3

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER:

DOCUMENT NUMBER:

139:7056

Regio and Stereoselective Ruthenium-Catalyzed Hydrovinylation of 1,3-Dienes: Application to the Generation of a 20(s) Steroidal Side Chain

AUTHOR(S):

CORPORATE SOURCE:

DOCUMENT SOURCE:

PUBLISHER:

DOCUMENT TYPE:

LANGUAGE:

COBSTRUCT OF THE AUTHOR OF

533922-77-8F RL: SPN (Synthetic preparation), PREP (Preparation) (regio- and stereoselective ruthenium-catalyzed hydrovinylation of 1,3-dienes, vinylcycloalkenes, and steroidal diene) 533925-77-8 CAPUS 4-Octen-7-3-1, 3-ethyl-7-[3-(phenylmethoxy)estra-1,3,5(10),16-tetraen-17-yl]-, (4E,7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

REFERENCE COUNT:

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued) study, unclassified), RCT (Reactant), SPN (Synthetic preparation), THU (Therapeutic use), BIOL (Biological study), PREP (Preparation), RACT (Reactant or reagent), USES (Uses) (lose) (aynthesis of cholestane compds. with a c17-alkyl side chain and arom. A-ring for use in cell modulating therapy) 305812-17-3 CAPLUS Acetamide, N-[(SR)-6-(3-hydroxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305812-18-4 CAPLUS 19-Norpregna-1,3,5(10),16-tetraen-3-ol, 20-{5-(ethylamino)-5-methylhexyl}-, (20R)- (9CI) (CA INDEX NAME)

305812-52-6 CAPLUS 19-Norcholesta-1,3,5(10)-trien-23-yne-3,25-diol (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN
SSION NUMBER: 2000:814500 CAPLUS
HENT NUMBER: 133:150095
E: Synthesis of cholestane compounds with a c17-alkyl side chain and an aromatic A-ring for use in cell modulating therapy
NTOR(S): Hesse, Robert Henry; Setty, Sundara Katugam Srinivasasetty; Ramgopal, Malathi; Kugabalusooriar, Sanga ACCESSION NUMBER: DOCUMENT NUMBER: TITLE: INVENTOR(S): Srinivassetty, Ramgopal, Malathi; Kugabalusocriar, Sanga Marsden, John, Christopher, UK; Research Institute for Medicine and Chemistry Inc. PCT Int. Appl., 75 pp. CODEN: PIXXD2 Patent English 1 PATENT ASSIGNEE (S): SOURCE: DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

WO 2000068246 Al 20001116 W0 2000-GB1813 20000511

W: AS, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CM, CR, CU, CZ, CZ, DE, DE, DK, OK, OM, OZ, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KR, KZ, LC, LX, LA, LS, IT, JU, LY, MA, MD, MG, MK, NM, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZV, AM, AZ, BY, KG, KP, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZY, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GM, GW, ML, MR, NE, SN, TD, TG

EP 1179005 Al 20020213 EP 2000-927569 20000511

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, TI, RO

ZA 2001005272 A 20021128 ZA 2001-9272 20011109

NO 2001005272 A 20021128 WO 2001-5520 20011112

PRIORITY APPLN. INFO.: GB 1999-10934 A 19990511

OTHER SOURCE(S): MARPAT 133:350395

AB Synthesis of cholestane compds. (I) (R1 and R2, which may be the same or different, = alkyl, alkenyl, alkynyl, R3 = Me having .alpha.— or .beta.—configuration, R4 = H or an etherifying or esterifying group, R5 = H, CH, alkoxy, X = OR4, wherein R4 is as defined above, or NRGR7 wherein R6 = H, aliph. or araliph. org. group linked to the nitrogen atom by way of a carbonyl group R7 = H, alkyl; Y = (Un)substituted alkylene, alkenylene, alkynylene; dotted lines signify that double bonds may be present at the 16(17)—position and/or either at the 6(7)—and (19)—positions or at the 7(8)—position] is disclosed for modulation of cell growth and differentiation, while having low calcemic activity. Thus, I [R1, R2 = Mer R3 = .alpha.—Mer R4, R5 = H; X = NHAC; Y = (CH2)44: .DELTA.16 double bondl is preped. by reaction of 3-triisopropolyliyloxyl-9-morchol-1,3,5(10),16—tetraene-24-bromide with acetonitrile followed by redn. of nitrile to amine, methylation of anine with Me lithium, acetylation of the amino wi

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN

305812-19-5P 305812-20-8P 305812-21-9P
305812-22-0P 305812-23-1P 305812-24-2P
305812-25-3P 305812-26-4P 305812-37-5P
305812-26-6P 305812-23-P 305812-30-0P
305812-31-1P 305812-32-2P 305812-33-3P
305812-31-1P 305812-33-8P 305812-33-9P
305812-37-7P 305812-33-8P 305812-39-9P
305812-40-2P 305812-41-3P 305812-48-P
305812-40-3P 305812-44-6P 305812-48-0P
305812-46-9P 305812-44-6P 305812-48-0P
305812-45-9P 305812-53-7P 305812-54-0P
305812-55-9P 305812-55-0P 305812-54-0P
305812-55-9P 305812-55-0P 305812-54-0P
305812-55-9P 305812-55-0P 305812-54-0P
305812-51-7P 305812-52-9P 305812-56-0P
305812-61-P3 305812-52-9P 305812-60-8P
305812-61-P3 305812-52-0P 305812-60-8P
305812-61-P3 305812-52-0P 305812-60-8P
305812-61-P3 305812-52-0P 305812-60-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified), SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of cholestane compds. with a c17-alkyl side chain and an arom. A-ring for use in cell modulating therapy)
305812-19-5 CAPLUS
19-Norpregna-1,3,5(10),16-tetraen-3-01, 20-(5-methyl-5-(methylamino)hexyl)-, (20R)- (9CL) (CA INDEX NAME)

305812-20-8 CAPLUS 19-Norpregna-1,3,5(10),16-tetraen-3-ol, 20-{5-(dimethylamino)-5-methylhexyl]-, (20R)- (9CI) (CA INDEX NAME)

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 305812-21-9 CAPLUS
CN 19-Norpregna-1, 3, 5(10), 16-tetraen-3-o1, 20-[5-(ethylmethylamino)-5methylhexyll-, (20R)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-22-0 CAPLUS
CN Acetamide, N-[(6R)-6-(3-methoxyestra-1,3,5(10),16-tetraen-17-y1)-1,1dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-23-1 CAPLUS
CN Acetamide, N-[(6R)-6-(3-ethoxyestra-1,3,5(10),16-tetraen-17-y1)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued

Absolute stereochemistry.

RN 305812-27-5 CAPLUS
CN Actamide, N-[(6R)-6-[(17.beta.)-3-hydroxyestra-1,3,5(10)-trien-17-y1]-1,1dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-28-6 CAPLUS CN 19,26,27-Trinoccholesta-1,3,5(10)-triene-3,24-diol, 24-(2-propynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry

RN 305812-29-7 CAPLUS
CN 19,26,27-Trinorcholesta-1,3,5(10)-triene-3,24-diol, 2-methoxy-24-(2-propynyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 305912-24-2 CAPLUS
CN Acetamids N-[(6R)-1,1-dimethyl-6-[3-(2-methylpropoxy)estra-1,3,5(10),16-tetraen-17-yl]heptyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-25-3 CAPLUS
CN Benzamide, N-[(6R)-6-(3-hydroxyestra-1,3,5(10),16-tetraen-17-y1)-1,1dimethylheptyl- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-26-4 CAPLUS
CN Benzeneacetamide, N-[(6R)-6-(3-hydroxyestra-1,3,5(10),16-tetraen-17-yl)1,1-dimethylheptyl]- (9C1) (CA INDEX NAME)

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued Absolute stereochemistry.

RN 305812-30-0 CAPLUS
CN 19,26,27-Trinorcholesta-1,3,5(10)-triene-3,24-diol, 24-(2-propynyl)-,
(205)- (9C1) (CA INDEX NAME)

Absolute stereochemistry

RN 305812-31-1 CAPLUS
CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(3-hydroxy-3-(2-propyny1)-1-hexen-5-ynyl]-, (20R) = (9C1) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

RN 305812-32-2 CAPLUS CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(3-hydroxy-3-(2-propynyl)-1-hexen-5-

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN ynyl]-2-methoxy-, (20R)- (9CI) (CA INDEX NAME) (Continued)

Absolute stereochemistry. Double bond geometry unknown.

305812-33-3 CAPLUS 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(3-hydroxy-3-(2-propynyl)-1-hexen-5-ynyl]-, (205)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

305812-34-4 CAPLUS 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethyl-2-hexynyl)-, (20R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued) 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethylhexyl)-, (20R)-(9C1) (CA INDEX NAME)

305812-30-8 CAPLUS
19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethylhexyl)-2-methoxy-, (20R)- (9CI) (CA INDEX NAME)

305812-39-9 CAPLUS 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethylhexyl)-, (205)-(3C1) (CA INDEX NAME)

305812-40-2 CAPLUS Acetamide, N-[(5R)-1,1-diethyl-5-{(17.beta.)-3-hydroxyestra-1,3,5(10)-trien-17-yl}-2-hexynyl]- (9CI) (CA INDEX NAME)

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN

(Continued)

305812-35-5 CAPLUS 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethyl-2-hexynyl)-2-methoxy-, (20R)- (9Cl) (CA INDEX NAME)

Absolute stereochemistry.

305812-36-6 CAPLUS 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethyl-2-hexynyl)-, (205)-(9C1) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-37-7 CAPLUS

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued) Absolute stereochemistry.

305812-41-3 CAPLUS Acetamide, N-[(58)-1,1-diethyl-5-[(17.beta.)-3-hydroxy-2-methoxyestra-1,3,5(10)-ttien-17-yl]-2-hexymyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305812-42-4 CAPLUS Acetamide, N-[(5S)-1,1-diethyl-5-[(17.beta.)-3-hydroxyestra-1,3,5(10)-trien-17-yl]-2-hexynyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305812-43-5 CAPLUS
19-Norpregna-1,3,5(10)-triene-20-methanol, .alpha.-(3-amino-3-ethyl-1-pentynyl)-3-hydroxy-, (205)- (9CI) (CA INDEX NAME)

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued) Absolute stereochemistry.

RN 305812-44-6 CAPLUS
CN 19-Norpregna-1,3,5(10)-triene-20-methanol, .alpha.-(3-amino-3-ethyl-1-pentyyl)-3-hydroxy-2-methoxy-, (205)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-45-7 CAPLUS CN 19-Norpregna-1,3,5(10)-triene-20-methanol, .alpha.-(3-amino-3-ethyl-1-pentynyl)-3-hydroxy-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued y1)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-49-1 CAPLUS
N 19,26,27-Trinorergosta-1,3,5(10),16-tetraen-3-ol, 24-amino-2-methomy-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-53-7 CAPLUS
CN 19-Norcholesta-1,3,5(10)-triene-3,25-diol (9CI) (CA INDEX.NAME)

Me R R H HO Me

RN 305812-54-8 CAPLUS
CN 19-Norcholesta-1,3,5(10)-trien-23-yne-3,25-diol, 2-methoxy- (9CI) (CA INDEX NAME)

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 305812-46-8 CAPLUS
CN Acetamide, N-[(GR)-6-(3-hydroxy-2-methoxyestra-1,3,5(10),16-tetraen-17-y1)1,1-dimethylheptyl]- (9Cl) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-47-9 CAPLUS CN 19-Norpregna-1,3,5(10),16-tetraen-3-o1, 20-(5-amino-5-methylhexyl)-2-methoxy-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-48-0 CAPLUS CN Acetamide, N-(3-hydroxy-2-methoxy-19-norcholesta-1,3,5(10),16-tetraen-25-

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued) Absolute stereochemistry.

RN 305812-55-9 CAPLUS CN 19-Norcholesta-1,3,5(10)-trien-23-yne-3,25-diol, (205)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-56-0 CAPLUS CN 19-Norcholesta-1,3,5(10)-triene-3,25-diol, 2-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-57-1 CAPLUS CN 19-Norcholesta-1,3,5(10)-triene-3,25-diol, 2-methoxy-, (205)- (9CI) (CA INDEX NAME)

L6 ANSWER 2 OF 3. CAPLUS COPYRIGHT 2003 ACS on STN (Continued) -

RN 305812-58-2 CAPLUS
CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(5-hydroxy-5-methyl-1,3-hexadienyl), (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

RN 305812-59-3 CAPLUS
CN 19-Norpregna-1,3,5(10),16-tetraen-3-o1, 20-(5-amino-5-methylhexyl)-,
(205)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-60-6 CAPLUS CN Acetamide, N-[(6S)-6-(3-hydroxyestra-1,3,5(10),16-tetraen-17-y1)-1,1-

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 AGS on STN (Continued) CN Acetamide, N-[(GR)-6-(3-hydroxysetra-1,3,5(10),6,16-pentsen-17-y1)-1,1-dimethylhepty1]- (9C1) (CA INDEX NAME)

. Absolute stereochemistry.

RN 305812-64-0 CAPLUS
CN 19-Morpregna-1,3,5(10),6,16-pentaen-3-o1,20-(5-amino-5-methylhexyl)-,
(20R) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 305813-30-3P 305813-32-5P 305813-36-9P 305813-38-1P 305813-41-6P 305813-43-8P 305813-44-PP 305813-46-1P 305813-47-PP 305813-51-8P 305813-55-2P 305813-55-2P 305813-55-5P 305813-55-5P 305813-55-5P 305813-55-5P 305813-55-6P RD: RCT (Reactant); SFN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (synthesis of cholestane compds. with a c17-alkyl side chain and arom. A-ring for use in cell modulating therapy)
RN 305813-30-3 CAPLUS
CN 19-Norpregna-1,3,5(10),16-tetraene-20-pentanamine, .alpha.,.alpha.dimethyl-3-[[tris(1-methylethyl)silyl]oxy]-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued) dimethylheptyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-61-7 CAPLUS
CN 19-Morcholesta-1,3,5(10),16-tetraen-3-ol, 25-amino-, (205)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-62-8 CAPLUS
CN Acetamide, N-[(205)-3-hydroxy-19-norcholesta-1,3,5(10),16-tetraen-25-y1](9C1) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-63-9 CAPLUS

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued

RN 305813-32-5 CAPLUS
CN Acetamide, N-[(6R)-1,1-dimethyl-6-[3-[[tris(1-methylethyl)silyl]oxy]estra1,3,5(10),16-teraen-17-yl]heptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 305813-36-9 CAPLUS
CN 19-Norpregna-1,3,5(10)-triene-20-pentanamine, .alpha..alpha.-dimethyl-3[{tris(1-methylethyl)sily1}oxy]-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 305813-38-1 CAPLUS
CN Acetamide, N-[(6R)-1,1-dimethyl-6-[(17.beta.)-3-[{tris(1-methylethyl)silyl]oxy}estra-1,3,5(10)-trien-17-yl]heptyl]- (9CI) (CA INDEX NAME)

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN

305813-41-6 CAPLUS
19.26,27-Trinorcholesta-1,3,5(10)-trien-24-01, 24-(2-propynyl)-3-[[tris(1-methylethyl)sily]loxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305813-43-8 CAPLUS 5-Octen-1-yn-4-ol, 4-{2-propynyl}-7-[(17.beta.)-3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10)-trien-17-yl]-, (7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

305813-51-8 CAPLUS Silane, [[25-[(triethylsilyl)oxy]-19-norcholesta-1,3,5(10)-trien-23-yn-3-yl]oxy]tris(1-methylethyl)- (9CI) (CA INDEX NAME)

305813-53-0 CAPLUS
3,5-Octadien-2-01, 2-methyl-7-[(17.beta.)-3-[[tris(1-methylethyl) silyl]oxy]estra-1,3,5(10)-trien-17-yl]-, (7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

305813-55-2 CAPLUS
19-Norpregna-1,3,5(10),16-tetraene-20-pentanamine, .alpha.,.alpha.dimethyl-3-[{tris(1-methylethyl)silyl]oxy}-, (20S)- (9CI) (CA INDEX NAME)

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

305813-44-9 CAPLUS 19-Norpregna-1, 3, 5(10) -triene-20-methanol, .alpha.-(3-amino-3-ethyl-1-pentynyl)-3-[[tris(1-methylethyl)silyl]oxy]-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305813-46-1 CAPLUS
19-Norpregna-1,3,5(10),16-tetraene-20-pentanamine, 2-methoxy.alpha.,alpha.-dimethyl-3-[{tris(1-methylethyl)silyl}oxy]-, (20R)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

 $\label{eq:capulos} \begin{tabular}{ll} 305813-47-2 & CAPLUS \\ Acetamide, & N-[(6R)-6-[2-methoxy-3-[\{tris(1-methylethyl)silyl]oxy]estral, 3,5(10), 16-tetraen-17-yl]-1, 1-dimethylheptyl]- (9CI) & (CA INDEX NAME) \\ \end{tabular}$ 

Absolute stereochemistry.

L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN Absolute stereochemistry. (Continued)

 $\label{lem:condition} 305813-56-3 \quad \text{CAPLUS} \\ \text{Acetamide, N-[(6S)-1,1-dimethyl-6-{3-[[tris(1-methylethyl)silyl]oxy]estral,3,5(10),16-tetraen-17-yl]heptyl}- (9CI) \quad (CA INDEX NAME) \\ \end{array}$ 

Absolute stereochemistry.

305813-58-5 CAPLUS
19-Norpregna-1,3,5(10),6,16-pentaene-20-pentanamine, .alpha.,.alpha.-dimethyl-3-[[tris(1-methylethyl)silyl]oxy]-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305813-59-6 CAPLUS Acetamide, N-[(6R)-1,1-dimethyl-6-[3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10),6,16-pentaen-17-yl]heptyl]- (9CI) (CA INDEX NAME)

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

REFERENCE COUNT:

THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT 10

L6 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1985:471583 CAPLUS
DOCUMENT NUMBER: 103:71583
A Stereoselective synthesis of 1,2-diols from
.alpha.-hydroxyaldehydes
AUTHOR(5): Dolence, E. Kutt; Adamczyk, Maciej, Watt, David S.,
Russell, Graeme B., Horn, Dennis H. S.
CORPORATE SOURCE: Dep. Chem., Univ. Byoning, Laramie, WY, 82071, USA
Tetrahedron Letters (1985), 26(9), 1189-92
CODEN: TELEAY; ISSN: 0040-4039
JOURNET TYPE:
LANGUAGE: English
The addn. of Lic.tplbond.COMe20-THP (THP = tetrahydro-2M-pyran-2-y1) to
(20R)-20-hydroxypregnane-20-carboxaldehydes I and II in the absence and in
the presence of BF3 afforded predominantly 20R,22R-diols III and IV or
20R,22S-diols V end VI, resp., characteristic of ecdysones.

IT 97452-83-00 97452-84-1p
RL: RCT (Reactant): SPN (Synthetic preparation), PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and hydrolysis-hydrogenation of)
RN 97452-83-0 CAPLUS
CN 19-Norcholesta-1,3,5(10)-trien-23-yne-20,22-diol, 3-methoxy-25[(tetrahydro-2Z-pyran-2-y1)oxy]-, (22R)- (9CI) (CA INDEX NAME)
Absolute stereochemistry.

Absolute stereochemistry.

97452-84-1 CAPLUS 19-Norcholesta-1,3,5(10)-trien-23-yne-20,22-diol, 3-methoxy-25-[(tetrahydro-ZH-pyran-2-yl)oxy]-, (22S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 3 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

97452-65-2P 97452-66-3P
RL: SPN (Synthetic preparation), PREP (Preparation)
(prepn. of)
97452-85-2 CAPLUS
19-Norcholectat-1,3,5(10)-triene-22,25-diol, 3-methoxy-, (22R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

97452-86-3 CAPLUS
19-Norcholesta-1,3,5(10)-triene-20,22,25-triol, 3-methoxy-, (225)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

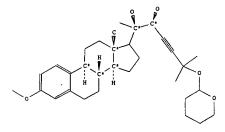
=> d all 1-4

09/926,491 Page 10

#### ANSWER 1 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN): CAS Reg. No. (RN): Chemical Name (CN): 4728055 97452-83-0, 97452-84-1 97452-03-0, 97452-04-1
2-(3-methoxy-13-methyl7,8,9,11,12,13,14,15,16,17-decahydro-6Hcyclopenta<apphenanthren-17-yl)-6-methyl-6(tetrahydro-pycan-2-yloxy)-hept-4-yne-2,3diol
2-(3-methoxy-13-methyl7,8,9,11,12,13,14,15,16,17-decahydro-6Hcyclopenta<apphenanthren-17-yl)-6-methyl-6(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3diol Autonom Name (AUN):

(tetrahydro-pyrar diol C32 H46 O5 510.71 71122, 6760, 289 Stereo compound heterocyclic 4263612 4567456 6-17 1991/12/02 Molec. Formula (MF):
Molecular Weight (MW):
Lawson Number (LN):
File Segment (FS):
Compound Type (CTYPE):
Constitution ID (CONSID):
Tautomer ID (TAUTID):
Beilstein Citation (BSO):
Entry Date (DED): Entry Date (DED): Update Date (DUPD): 1991/12/02



#### Field Availability:

Code	Name	Occurrence
***	*****	
BRN	Beilstein Records	1
RN	CAS Registry Number	2
CN	Chemical Name	1
AUN	Autonomname	1

# L7 ANSWER 1 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN (Continued) Reactant (.RCT): 2-(3-methoxy-13-methyl-

2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta(a>phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-

1013 (did)
472203
2 (3-methoxy-13-methyl7,8,9,11,12,13,14,15,16,17-decahydro-6Hcyclopenta(a>phenanthren-17-yl)-6-methylhept-4-yne-2,3,6-triol

No. of React. Details (.NVAR):

Reaction Details:

Reaction RID (.RID): 2742338.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 90 percent (BRN=4722039)
Reagent (.RGT): 70 percent HCLO4
Solvent (.SOL): H2O, methanol
Reference(s):
1. Dolence, E. Kurt; Adamczyk, Haciej; Watt, David S.; Russell, Graeme B.;
HOrn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>,
1189-1192; BABS-5554079

### Reaction:

Reaction ID (.ID): Reactant BRN (.RBRN): Reactant (.RCT): 2742337 4728055

2-(3-methoxy-13-methy)7, 8, 9, 11, 12, 13, 14, 15, 16, 17-decahydro-6Hcyclopentaxa>phenanthren-17-y1)-6-methyl-6(tetrahydro-pyran-2-yloxy)-hept-4-yne-2, 3-

diol 4722038

Product BRN (.PBRN): Product (.PRO):

2-(3-methoxy-13-methy)-7,8,9,11,12,13,14,15,16,17-decahydro-GH-cyclopentaxa3phenanthren-17-y1)-6-methyl-hept-4-yne-2,3,6-triol

No. of React. Details (.NVAR):

### Reaction Details:

Reaction RID (.RID): 2742337.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 90 percent (BRN=4722038) 70 percent HCLO4
Solvent (.SOL): H2O, methanol
Reference(s): 1. Dolence, E. Kurt; Adamczyk, Haciej; Watt, David S.; Russell, Graeme B.;
HOrn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>, 1189-1192; BABS-5554079

ANSWER 1 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Molecular Formula Formular Weight Lawson Number File Segment Compound Type Constitution ID Tautomer ID Beilstein Citation Entry Date Update Date IN
FS
CTYPE
CONSID
TAUTID
BSO
ED
UPD

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	
RXREA	Substance is Reaction Reactant	:
RXPRO	Substance is Reaction Product	

## Reaction: RX

Reaction ID (.ID): Reactant BRN (.RBRN): Reactant (.RCT):

2442472 4525023, 4133964

Product BRN (.PBRN): Product (.PRO):

2-14/2 4252023, 4133964 2-hydroxy-2-(3-methoxy-13-methyl-7,8,9,11,21,31,14,15,16,17-decahydro-6H-cyclopenta(a)phenanthren-17-yl)-propionaldehyde, C10H15BrHgO2 4728055, 4728054 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta(a)phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol, 2-(3-methoxy-13-methyl-7,8,9,11,21,31,14,15,16,17-decahydro-6H-cyclopenta(a)phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol

No. of React. Details (.NVAR):

## Reaction Details: RX

Reaction RID (.RID): 2442472.1
Reaction Classification (.CL): Preparation
Solvent (.SOL): tetrahydrofuran
-26 Cel
Note(s) (.COM): Yield given. Yields of byproduct given
Reference(s): 1. Dolence, E. Xurt, Adamczyk, Maciej; Watt, David S., Russell, Graeme B.;
Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>,
1189-1192; BABS-5554079

### Reaction: RX

Reaction ID (.ID): Reactant BRN (.RBRN): 2742338

#### L7 ANSWER 2 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN): CAS Reg. No. (RN): Chemical Name (CN):

2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<aphenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-

Autonom Name (AUN):

7, 8,9,11,12,13,14,15,16,17-decahydro-6H-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopents<apphenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-ylaxy)-hept-4-yne-2,3-

(tetrahydro-pyran diol C32 H46 O5 510.71 17122, 6760, 289 Stereo compound heterocyclic 4263612 4567455 6-17 1991/12/02 1991/12/02 Molec. Formula (MF): Molecular Weight (MW): Lawson Number (LN): File Segment (FS): Compound Type (CTYPE): Constitution ID (CONSID): Tautomer ID (TAUTID): Beilstein Citation (BSO): Entry Date (DED):

Entry Date (DED): Update Date (DUPD):

### Field Availability:

Code	Name	Occurrence
======	************************	
BRN	Beilstein Records	1
RN	CAS Registry Number	2
CN	Chemical Name	1
AUN	Autonomname	. 1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
FS	File Segment	ī

L7 ANSwar. (Continued) CTYPE

CONSID

```
Compound Type
Constitution ID
Tautomer ID
Beilstein Citation
            TAUTID
            BSO
           ED
UPD
                                  Entry Date
Update Date
       This substance also occurs in Reaction Documents:
           Code
            RX
RXPRO
                                  Reaction Documents
Substance is Reaction Product
Reaction:
RX
                                                                                   2442472
4525023, 4133964
2-hydroxy-2-(3-methoxy-13-methyl-
7,8,9,11,12,13,14,15,16,17-decahydro-6H-
cyclopenta-aphenanthren-17-41)-
propionaldehyde, C10H15BrMgO2
4728055, 4728054
4728055, 4728054
7,8,9,11,12,13,14,15,16,17-decahydro-6H-
cyclopenta-aphenanthren-17-y1)-6-methyl-6-
(tatrahydro-pyran-2-yloxy)-hept-4-yne-2,3-
diol, 2-(3-methoxy-13-methyl-
7,8,9,11,12,13,14,15,16,17-decahydro-6H-
cyclopenta-aphenanthren-17-y1)-6-methyl-6-
(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-
diol
          Reaction ID (.ID):
Reactant BRN (.RBRN):
Reactant (.RCT):
           Product BRN (.PBRN):
Product (.PRO):
          No. of React. Details (.NVAR):
Reaction Details:
          Reaction RID (.RID): 2442472.1
Reaction Classification (.CL): Preparation
Solvent (.SOL): tetrahydrofuran
-26 Cel
Note(s) (.COM): Yield given. Yields of byproduct given
Reference(s): Yield given. Yields of byproduct given
Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>,
1189-1192; BABS-5554079
          ANSWER 3 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)
CONSID
TAUTID
                                  Constitution ID
                                  Tautomer ID
Beilstein Citation
            BSO
            ED
                                  Entry Date
           UPD
                                  Update Date
Nuclear Magnetic Resonance
       This substance also occurs in Reaction Documents:
           Code
                                                                                                                Occurrence
            RX
RXPRO
                                  Reaction Documents
Substance is Reaction Product
Nuclear Magnetic Resonance:
           Description (.KW):
                                                                                    Chemical shifts
13C
            Nucleus (.NUC):
Solvents (.SOL):
                                                                                    pyridine-d5
           Reference(s):
1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.;
Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>,
1189-1192; BABS-5554079
Reaction:
RX
          Reaction ID (.ID):
Reactant BRN (.RBRN):
Reactant (.RCT):
                                                                                     2737115
4722039
                                                                                    4722039
27.2039
27.2039
27.8.9.11.12.13.14.15.16.17-decahydro-6H-
cyclopenta<a>phenanthren-17-y1)-6-methyl-
hept-4-yne-2,3,6-triol
4719751
         ### 4719751 | 4719751 | 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta/asphenanthren-17-yl)-6-methyl-heptane-2,3,6-triol
Reaction Details:
RX
          Reaction RID (.RID): 2737115.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): Pto2
Catalyst (.CAT): Pto2
           Reference(s):
1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.;
Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>,
1189-1192; BABS-5554079
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ANSWER 2 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

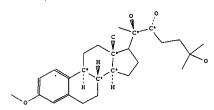
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ANSWER 3 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
   Beilstein Records (BRN):
Beilstein Pref. RN (BPR):
CAS Reg. No. (RN):
Chemical Name (CN):
                                                                                                                          7-452-96-3
2-(3-methoxy-13-methyl-
7,8,9,11,12,13,14,15,16,17-decahydro-6H-
cyclopenta<a>phenanthren-17-yl)-6-methyl-
heptane-2,3,6-triol
2-(3-methoxy-13-methyl-
7,8,9,11,12,13,14,15,16,17-decahydro-6H-
cyclopenta<a>phenanthren-17-yl)-6-methyl-
heptane-2,3,6-triol
C27 H2 O4
430.63
6704, 299
Stereo compound
isocyclic
4257631
4555354
   Autonom Name (AUN):
  Molec. Formula (MF):
Molecular Weight (MW):
Lawson Number (LN):
File Segment (FS):
Compound Type (CTYFE):
Constitution ID (CONSID):
Tautomer ID (TAUTID):
Beilstein Citation (BSO):
Entry Date (DED):
Update Date (DUPD):
                                                                                                                                4555354
                                                                                                                              6-06
1991/12/02
1993/03/20
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#### Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	. 1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1

L7 ANSWER 4 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN): Beilstein Pref. RN (BPR): CAS Reg. No. (RN): Chemical Name (CN): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopentacaphenanthren-17-yl)-6-methyl-heptane-2,3,6-triol heptane-2, 3, 6-triol
2-(3-methoxy-13-methyl7,8,9,11,12,13,14,15,16,17-decahydro-6Hcyclopenta-4>phenanthren-17-yl)-6-methylheptane-2,3,6-triol
C27 H42 0
430.63
6704, 289
Stereo compound
isocyclic
4257631
4255533 Autonom Name (AUN): Molec. Formula (MF):
Molecular Weight (MW):
Lawson Number (LN):
File Segment (FS):
Compound Type (CTYFE):
Constitution ID (CONSID):
Tautomer ID (TAUTID):
Beilstein Citation (BSO):
Entry Date (MEN): 4555353 6-06 1991/12/02 1993/03/20 Entry Date (DED): Update Date (DUPD):



#### Field Availability:

Name	Occurrence
Beilstein Records	1
Beilstein Preferred RN	1
CAS Registry Number	1
Chemical Name	1
Autonomname	1
Molecular Formula	1
Formular Weight	1
Lawson Number .	2
File Segment	1
Compound Type	1
D Constitution ID	1
D Tautomer ID	1
Beilstein Citation	1
Entry Date	1
	Beilstein Records Beilstein Preferred RN CAS Registry Number Chemical Name Autonomname Molecular Formula Formular Weight Lawson Number File Segment Compound Type Constitution ID Tautomer ID Beilstein Citation

```
L7 ANSWER 4 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN (Continued)

UPD Update Date
NMR Nuclear Magnetic Resonance 1

This substance also occurs in Reaction Documents:

Code Name Occurrence
RX Reaction Documents 1

RMPRO Substance is Reaction Product 1

Nuclear Magnetic Resonance:
NMR
Description (.KW): Chemical shifts
Nucleus (.NUC): 13C
Solvents (.SOL): pyridine-d5
Reference(s): 1. Dolence, E. Kurt, Adamczyk, Maciej, Watt, David S., Russell, Graeme B., Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>, 1189-1192, BABS-5554079

Reaction:
RX
Reaction ID (.ID): 2737114
Reaction ID (.RDN): 4722038
Reaction (.RCT): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta(a>phenanthren-17-yl)-6-methyl-hept-4-yne-2,3,6-triol
Product BRN (.PBRN): 4719750
Product (.PRO): 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta(a>phenanthren-17-yl)-6-methyl-hept-4-yne-2,3,6-triol
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 2737114.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): H2
Reaction Classification (.CL): Preparation
Reagent (.RGT): H2
Reaction Classification (.CL): Preparation
Reagent (.RGT): H2
Reference(s): 1. Dolence, E. Kurt, Adamczyk, Haciej, Watt, David S., Russell, Graeme B., Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>, 1189-1192; BABS-5554079
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09/926,491 Page 13

=> d ibib ab fqhit 1-14

09/926,491 L9 ANSWER 1 OF 14 HARPAT COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 138:73420 HARPAT
TITLE: Preparation of anti-estrogenic steroids, and
associated pharmaceutical compositions and methods of use Tanabe, Masato: Peters, Richard H.; Chao, Wan-Ru; INVENTOR (S): Jong, Ling SRI International, USA U.S., 50 pp., Cont. of U.S. Ser. No. 220,408. CODEN: USXXXAM PATENT ASSIGNEE(S): SOURCE: DOCUMENT TYPE: Patent English 4 FAMILY ACC. NUM. COUNT: PATENT INFORMATION: PATENT NO. KIND DATE APPLICATION NO. DATE US 6503896 B1 20030107
US 6054446 A 2000425
EP 1310509 A2 20030514
R: DE, FR, GB, IT, NL
US 6281205 B1 20010828
PRIORITY APPLN. INFO.: US 2001-872826 US 1997-998877 EP 2003-183 R: DE, FR, GB, IT, NL
US 6281205 B1 20010828 US 1998-220408 19981224

RITY APPLN. INFO.:
US 1998-220408 19981224

US 1998-220408 19981224

US 1998-220408 19981224

EP 1998-964882 19981223

Steroid derivs., such as I and II [R = C, N, dashed lines = optional double bond; X, X1 = hydrocarbyl, generally including at least one O, S, N atom in the form of -O-, -S-, -NH- or, -N(alkyl)-linkage; XX1 = heterocyclic ring; R1 = H, alkyl; R2 = H, OH, alkyl, alkoxyl, thioalkyl; R3-R5, R7, R9 = H, alkyl; R6 = H, OH, alkyl, alkoxyl, thioalkyl; R3-R5, R7, R9 = H, alkyl; R6 = H, OH, alkyl, alkoxyl, thioalkyl; R3-R5, R7, R9 = H, alkyl; R6 = H, OH, alkyl, alkoxyl, thioalkyl; R2 = H, CH, alkyl; R2 = H, OH, alkyl; R10 = Me, Et; R20 = :CH(CH2)m-On-L-(CH2)m-NR2!R22; c-O-6; L = cyclic or heterocyclic ring; R21, R22 = alkyl; R2!R22 = cycloalkyl, heterocycloalkyl], or a pharmaceutically acceptable salt thereof, were prept to treat a variety of disorders, particularly estrogen-dependent disorders including prostatic cancer. Thus, (E)-3-hydroxy-21-[2'-(piperazinyl)ethoxy]-19-norpregna-1,3,5(10),17(20)-tetraene (III) was prepd. via a multistep synthetic sequence starting from estrone, vinylmagnesium bromide, and 1-(2-hydroxysthyl)piperazine. III exhibited 1003 antiestrogenic activity against Ruman ishikawa cells at 10 .mu. M concn. Therapeutic methods and pharmaceutical compns. were also provided. 19981223 MSTR 3 L9 ANSWER 2 OF 14 MARPAT COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:
137:370278 MARPAT
137:370278 MARPAT
137:370278 MARPAT
Preparation of substituted pregna-1,3,5(10)-triene
derivatives for pharmaceutical use
derivatives for pharmaceutical use
ferse, Robert Henry Setty, Sundara Katugam
Srinivasasetty; Pechet, Maurice Murdoch; Gile, Michael
Marsden, John Christopher, UK; Research Institute for
Medicine and Chemistry Inc.
PCT Int. Appl., 28 pp.
COODEN: PIXXD2
DOCUMENT TYPE:
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION: DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: PATENT INFORMATION:

PATENT NO. KIND DATE

APPLICATION NO. DATE

WO 2002092100 A1 AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CC, CR, CU, CZ, DB, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, DF, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, NM, MM, MX, MZ, NM, NN, ZO, MP, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VM, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FT, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CT, CM, GA, GM, GD, GW, ML, MR, MZ, SN, TD, TG

PRIORITY APPLN. INFO:

US 2001-290013F 20010511

AB Pregna-1,3,5(10)-triene derivs., such as I (RI = H, hydroxy protecting group; R2 = GH, CHO, alkowy, alkenyl, alkyl, etc.; R3 = .alpha.-,
.beta.-Me; X = Cl-3 alkylene group, bond; Y = CR4| (RS)NR67; R4, R5 = H, alkyl, alkenyl and alkynyl groups, such that the total carbon content of R4 and R5 does not exceed three atoms R6 = H, aliph. or araliph. org. group, acyl, etc.; Cl6-C17 = satd., unsatd.), were prepd. for a variety of therapeutic uses, such as modulating cell activity, including antiproliferative and antiangiogenic effects. Thus, pregna-1,3,5(10)-triene derivs. II (Y = NN2, NHCOMe) were prepd, via a multistep synthetic series starting from 2-methoxy-3-[[tris(1-methylethyl)silyl]oxy]-estra-1,3,5(10)-trien-17-one and ethyltriphenylphosphonium bromide.
Pharmaceutical compns. of the prepd. compds. were discussed, but specific pharmaceutical activity testing data was not presented.

> - OH - OH - alkylene<(1-3)> - 30

```
L9 ANSWER 1 OF 14 MARPAT COPYRIGHT 2003 ACS on STN (Continued)

G4 - 28

G5

G7 - OH
G24 - Me
G41 - 106

G43-G44

106

G47

G43 - Ak (SO)
G47 - alkyl<(1-24)> (SO)
DER: or pharmacountically acceptable salts or esters
MPL: disclosure
NTE: oxo substitution also disclosed

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
```

L9 ANSWER 2 OF 14 MARPAT COPYRIGHT 2003 ACS on STN (Continued)

G8 = alky1<(1-3)>
G8 = nH2
MPL: claim 1
NTE: total carbon carbon content of G8 does not exceed three atoms when the substitution is restricted

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

(Continued)

```
L9 ANSWER 3 OF 14 MARPAT COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 137:47357 MARPAT
TITLE: Preparation of 2-methoxyestradiol derivatives as antianglogenic agents
Agoston, Gregory E.; Shah, Jamshed H.; Hunsucker, Kimberly A.; Pribluda, Victor S.; Lavallee, Theresa M.; Green, Shavn J.; Herbstritt, Christopher J.; Zhan, Xiaoguo H.; Treston, Anthony M.
USA U.S. Pat. Appl. Publ., 37 pp., Cont.-in-part of U.S. Ser. No. 933,894.
CODEN: USXXCO
DOCUMENT TYPE: Patent INFORMATION:
English
FAMILIY ACC. NUM. COUNT: PATENT INFORMATION:
                      DOCUMENT TYPE:
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
                                                        PATENT NO. KIND DATE APPLICATION NO. DATE

US 2002082433 A1 20020627 US 2001-939208 20010824

RITY APPLM. INFO.: US 2000-641327 20000618

US 2000-2553385 20001127

US 2000-255302P 20001213

US 2000-255302P 20001213

US 2001-933894 20010823

2-Methoxyestradiol derivs. of formula I (R1, R4 = H, halo, CM, alkyl, OH, NH2, etc.: R2 = N3, CN, OMe, alkenyl, alkynyl, alkowy, NH2, etc.: R3. = OH, OAC: R5 = alkyl, alkenyl, (di)alkylamino, OH, alkylane, etc.: R6, R7 = H, alkyl, alkenyl, alkynyl, halo, etc.] are prepd. for treating mammalian disease characterized by undesirable angiogenesis. Thus, II was prepd. for Teating mammalian disease characterized by undesirable angiogenesis. Thus, II was prepd. for Teating mammalian disease characterized by undesirable angiogenesis. Thus, II was prepd. for Teating mammalian disease characterized by undesirable angiogenesis. Thus, II was prepd. for Teating mammalian disease characterized by undesirable angiogenesis. Thus, II was prepd. from 2-methoxyestradiol and propyltriphenylphosphonium bromide. The ICSO of II against MDA-MB-231 breast tumor cells was 51.31 .mu.M.
                    US 2002082433
PRIORITY APPLN. INFO.:
                                                                                                     alkoxy<(-10)> (SO (1-) F)
                      ម្ពç---G13
                                                                            - alkyl<(1-10)> (SO (1-) G21)
- CF3 / OH
claim 1
               L9 ANSWER 4 OF 14
ACCESSION NUMBER:
TITLE:

INVENTOR(S):

Agoston, Gregory: Shah, Jamshed H., Hunsucker,
Kimberly A., Pribluda, Victor: Lavallee, Theresa M.,
Green, Shawn J., Herbstritt, Christopher J., Zhan,
Xiaoguo H., Treston, Anthony

PATENT ASSIGNEE(S):
SOURCE:

DOCUMENT TYPE:
LANGUAGE:
PIXED2
PATENT INFORMATION:

DOCUMENT TYPE:
LANGUAGE:
PIXED2
PATENT INFORMATION:
PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

**CO2002042319 A2 20020530 W0 2001-US26490 20010824

W0 2002042319 A3 20030313

**E' AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DZ, DK, DM, DZ, EC, EZ, ES, FI, GB, GD, GE, GH, CM, EB, HU, 1D, LI, IN, IS, JF, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LY, MA, HD, MG, MK, HN, MW, MK, MZ, NO, MZ, PH, PL, PT, NO, NU, SD, SE, SG, SI, SS, TS, TJ, TH, TR, TT, TZ, UA, UG, US, UZ, VM, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RY: GH, GM, KE, LS, MW, MZ, SD, SI, SZ, TZ, GG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GM, GG, GW, ML, MR, NE, NN, TD, TG

AU 200108386 AS 20020603 AU 2001-89896 20010824

EP 1343803 A2 20030917 EP 2001-968112 20010824

EP 1343803 AZ 20030917 EP 2001-968112 20010824

EP 1347804 AT, BE, CR, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

US 2000-255302P 20001273

US 2001-278250P 2001023

WO 2001-US26490 20010824

AB 2-Methoxyestradiol analogs, such as I [R], R3 = H, halo, CM, alkyl, OH, CH2OH, NH2, alkynl, alkynyl, vere prepd for treating mammalian disease characterized by undesirable angiogenesis. Thus, 2-methoxyestradiol analog II was prepd. by the reaction of methyltriphenylphosphonium bromide and 2-methoxyestrone. In vitro evaluation against MDA-MB-231 breast tumor cells and MUVEC endothelial cells, II showed IC50 0.24.+-.0 and 0.19.+-0.19 resp.
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L9 ANSWER 4 OF 14 MARPAT COPYRIGHT 2003 ACS on STN
                                                                            (Continued)
         - alkoxy<(-10)> (SO (1-) F)
ĦĞ-
     -G13
        - alkyl<(1-10)> (50 (1-) G21)
- CF3 / OH
claim 1
additional double bond formation also claimed
```

ANSWER 3 OF 14 MARPAT COPYRIGHT 2003 ACS on STN additional double bond formation also claimed

L9 ANSWER 5 OF 14
ACCESSION NUMBER:
TITLE: Preparation of novel anti-estrogenic steroids
INVENTOR(S): Jong, Ling
PATENT ASSIGNEE(S): USA
SOURCE: USA
COURENT TYPE: COURT TYPE:
LANGUAGE: English English LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: PATENT NO. APPLICATION NO. KIND DATE DATE 20020314 20030415 20000425 20030514 US 2002032180 US 6548491 US 6054446 EP 1310509 A1 B2 US 2001-872825 20010531 US 1997-998877 EP 2003-183 19971224 19981223

US 6054446 A 20030415
EP 1310509 AZ 20030514
R: DE, FR, GB, IT, NL
US 6281205 B1 20010828
US 2003153543 A1 20030814
PRIORITY APPLN. INFO.:

R: DE, FR, GB, IT, NL

US 6281205 Bl 20010828 US 1998-220408 19981224

US 2003153543 Al 20030814 US 2002-327401 20021219

ORITY APPLN. INFO:

US 1998-220408 19981224

EP 1998-964881 19981223

Novel antiestrogenic compds., e.g. of formula I [X - Mydrocarbon contg. O, S or N, etc.; XX1 = H, hydrocarbon contg. O, S or N, etc.; XX1 = H, alkyl, halo, etc.; R2 = H, OH, etc.; R3 = H, OH, CN, alkyl, etc.; R4 = H, alkyl, r8, etc.; R5 = H, alkyl, r8, etc.; R6 = H, OH, etc.; R8 = H, OH, etc.; R9 = H, alkyl; R7 = H, halo, nitro, CHO, allyl, etc.; R8 = H, OH, etc.; R9 = H, alkyl; R7 = H, halo, nitro, CHO, allyl, etc.; R8 = H, OH, etc.; R9 = H, alkyl; R7 = H, halo, nitro, CHO, allyl, etc.; R8 = H, OH, etc.; R9 = H, alkyl; R10 = Me, Et], are preped, which are useful to treat a variety of disorders, particularly estrogen-dependent disorders. Preferred compds. have a 1,3,5-estratrien nucleus, and are substituted at the C-17 or C-11 position with a mol. moiety which renders the compds. effective to competitively block the binding of estrogen to its receptor. Therapeutic methods and pharmaceutical compns. are provided as well. Thus, II citrate salt was prepd. from 7.alpha.-methyl-17.beta.-hydroxyethyl-1,3,5-estratrien-3-ol, vanilin and diethylamine. II citrate salt showed significant growth suppressive activity against MCF-7 tumor in mice at 10 mg/kg/day.

#### METR 3

L9 ANSWER 6 OF 14 MARPAT COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER:

TITLE: 135:358085 MARPAT
Preparation of 2-substituted pregna-1,3,5(10)-triene and chola-1,3,5(10)-triene derivatives with antiproliferative and antiangiogenic activity
Hesse, Robert Henry Setty, Sundara Katugam
Srinivasasetty, Pechet, Maurice Murdoch; Gile, Michael
Marsden, John Christopher, UK; Research Institute for Medicine and Chemistry Inc.

SOURCE: PCT Int. Appl., 40 pp.
CODEN: PIXKUS

DOCUMENT TYPE: Patent
LANGUAGE: English

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: English 1

ANSWER 5 OF 14 MARPAT COPYRIGHT 2003 ACS on STN (Continued)

= 23

`G31

Ħ6-

G24 G25 G27 G31

- OH - Me - Ak (SR (1-) G26) - O - alkyl<(1-24)> claim 20 - pharmaceutics

or pharmaceutically acceptable salts or esters

ANSWER 6 OF 14 MARPAT COPYRIGHT 2003 ACS on STN

alkyl<(1-3)> claim 1 total carbon carbon content of G8 does not exceed three atoms substitution is restricted

THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

(Continued)

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L9 ANSWER 7 OF 14 MARPAT COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 135:195698 MARPAT
TITLE: Preparation of anti-estrogenic steroids, and
associated pharmaceutical compositions and methods of
                                                                          use
Tanabe, Masato; Peters, Richard H.; Chao, Wan-ru;
Jong, Ling
Sri International, USA
U.S., 50 pp., Cont.-in-part of U.S. 6,054,446.
CODEN: USXXAM
Patent
English
4
  INVENTOR (S):
  PATENT ASSIGNEE(S):
SOURCE:
 DOCUMENT TYPE:
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
                PATENT NO.
                                                                                 DATE
                                                                                                                              APPLICATION NO.
US 6281205 B1 20010828
US 6054446 A 20000425
EP 1910509 A2 20030514
R: DE, FR, GB, IT, MI
US 2002032180 A1 20020314
US 6548491 B2 20030151
US 650869 B1 20030107
US 2002032181 A1 20020314
US 6455517 B2 20020924
US 2003153543 A1 20030814
PRIORITY APPLN. INFO.:
                                                                                                                              US 1998-220408
US 1997-998877
EP 2003-183
                                                                                                                                                                                19981224
19971224
19981223
                                                                                                                                                                                20010531
                                                                                                                              US 2001-872825
                                                                                                                              US 2002-327401
US 1997-998877
EP 1998-964882
US 1998-220408
US 2001-872825
```

Us 2001-872825 20010531

Novel antiestrogenic compds. are prepd. which are useful to treat a variety of disorders, particularly estrogen-dependent disorders. Preferred compds. have a 1,3,5(10)-estratriene nucleus, and are substituted at the C-17 or C-11 position with a mol. moiety which renders the compds. effective to competitively block the binding of estrogen to its receptor. Particularly preferred compds. are 17-desoxy-1,3,5(10)-estratrienes, e.g. of formula I [R] = H, alkoxy, halo, CN, etc.; R2 = H, OH, alkyl, etc.; R3 = H, alkyl, acyl, S02MHz, etc.; R4, R5 = H, alkyl, heterocyclyl; etc.; L = (substituted) five- or six-membered cyclic moiety; m = 1-6; p = 0-6]. Thus, II citrate salt was prepd. and showed strong growth inhibitory activity against MCF-7 human mammary tumor at 10 mg/kg/day. Therapeutic methods and pharmaceutical compns. are provided as well.

```
DOCUMENT TYPE:
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
                                                                                                                                                                                                                               APPLICATION NO. DATE
... R., DE, CH, DE, DX, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

2A 2001009272 A 20021128 ZA 2001-9272 20011109
NO 2001005520 A 20020109 NO 2001-5520 20011112
RRITY APPLN. INFO.:
GB 1999-10934 19990511
WO 2000-GB1813 20000511
Synthesis of cholestane compds. (I) [Rl and R2, which may be the same or different, = alkyl, alkenyl, alkynyl; R3 = Me having .alpha.- or .beta.-configuration; R4 = H or an etherifying or esterifying group; R5 = H, OH, alkoxy; X = OR4, wherein R4 is as defined above, or NRGR7 wherein R6 = H, aliph. or araliph. org group, average and aliph. araliph. or aryl org. group inked to the nitrogen atom by way of a carbonyl group; R7 = H, alkyl; Y = (un) substituted alkylene, alkenylene, alkynylene; dotted lines signify that double bonds may be present at the 16(17)-position and/or either at the 6(7)- and 8(9)-positions or at the 7(8)-position) if disclosed for modulation of cell growth and differentiation, while having low calcende activity. Thus, I [R1, R2 = Me; R3 = .alpha.-Me; R4, R5 = H; X = NHAC; Y = (CH2)4; DELTA.16 double bond) is prepci. by treation of attrisopropylsilyloxy-19-norchol-1,3,5(10),16-tatraene-24-bromide with acetonicitile followed by read. of nitrile to amine, methylation of amine with Me lithium, acetylation of the amino with acetic anhydride and desilylation with TBAF.
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ANSWER 7 OF 14 MARPAT COPYRIGHT 2003 ACS on STN G12 d19 622 - 23 赆 G31 - 28 ĀĈ--G5 G17 G24 G25 G27 G31 - OH - Me - Ak (SR (1-) G26) - O - alkyl<(1-24)> claim 3 or pharmaceutically acceptable salts or esters oxo substitution also claimed also incorporates broader disclosure NTE:

ANSWER 8 OF 14 MARPAT COPYRIGHT 2003 ACS on STN

- loweralkyl

- OH - loweralkylene (SO G10)

OH claim 1

REFERENCE COUNT:

REFERENCE COUNT:

THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 10 OF 14 MARPAT COPYRIGHT 2003 ACS on STN

131:88084 MARPAT

TITLE: Preparation of novel antiestrogenic steroids

Tanabe, Masato; Peters, Richard H.; Chao, Wan-Ru;

Jong, Ling

PATENT ASSIGNEE(S): SRI International, USA

PCT Int. Appl. 142 pp.

CODEN: PIXXD2

PATENT TYPE: LANGUAGE: Patent

LANGUAGE: PATENT NO. KIND DATE APPLICATION NO. DATE

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

WO 9933859 A2 19990708 WO 1998-USZ7406 19981223

W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE,

DK, EE, ES, FI, 6B, GE, GH, 6M, HR, HU, ID, IL, IN, IS, JP, KE,

KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW,

MC, NO, NO, NZ, PL, PT, RO, RU, SD, SE, 5G, SI, SK, SK, LT, JT, HT,

TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES,

FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BP, BJ, CF, CG, CI,

CM, GA, GW, ML, MR, MR, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES,

FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BP, BJ, CF, CG, CI,

CM, GA, GW, ML, MR, ME, SD, SZ, CH, ZW, AT, BE, CH, CY, DE, DK, ES,

FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BP, BJ, CF, CG, CI,

CM, GA, WG, ML, MR, MR, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES,

FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BP, BJ, CF, CG, CI,

CM, GA, SY, NL, MR, MR, NE, SD, SZ, CH, ZW, AT, BE, CH, CY, DE, DK, ES,

FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BP, BJ, CF, CG, CI,

CM, GA, SY, NL, MR, MR, NE, SD, SZ, CH, ZW, AT, BE, CH, CY, DE, DK, ES,

FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BP, BJ, CF, CG, CI,

CM, GA, SW, ML, MR, NE, SD, SZ, CH, SW, AT, BE, CH, CY, DE, DK, ES,

FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BP, BJ, CF, CG, CI,

CM, GA, SW, SW, SS, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES,

FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BP, BJ, CF, CG, CI,

CM, GA, SW, SW, SS, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES,

FI, FR, GB, TN, MR, SD, SZ, CU, ZW, AT, BE, CH, CY, DE, DK, ES,

FI, FR, GB, TN, MR, SD, SZ, CU, ZW, AT, BE, CH, CY

L9 ANSWER 9 OF 14 MARPAT COPYRIGHT 2003 ACS on STN (Continued)

G5 G6
G5 G1
G5 G2
G3 = alkoxy<(1-20)>
G6 = hydrocarbyl<(2-14)> (SO (1-) G7)
G7 = CO2H / alkoxy<(1-3)> / alkyl<(1-5)>
G11
G11
MPL: claim 3

L9 ANSWER 10 OF 14 MARPAT COPYRIGHT 2003 ACS on STN (Continued)

G13
G2
G4
G14
G13
G19
G22
G3
G3
- 23
G25
G25
G27
G4
G64
G17
G28
G27
G31
G4
- 28
HC
G26
G27
G31
G31
G4
- 28
HC
G27
G31
G31
G4
- 28
HC
G28
G31
G4
- 28
HC
G29
G31
G4
- 28
HC
G21
G31
- OH
G24
- Me
G25
- Ak (SR (1-) G26)
G27
G31
- alkyl<(1-24)>
or pharmaceutically acceptable salts or esters or pharmaceutically acceptable salts or esters
HDL: claim 20
NTE: oxo substitution also claimed

L9 ANSWER 11 OF 14 MARPAT COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 122:81747 MARPAT
TITLE: Preparation of polyaminosteroids as bactericides and antifungals
INVENTOR(S): Frye, Leah L., Zasloff, Michael A., Kinney, William A., Moriarty, Robert M.
PATENT ASSIGNEE(S): Magainin Pharmaceuticals Inc., USA
PCT Int. Appl., 129 pp.
COUNENT TYPE: Patent
LANGUAGE: English

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: English 5

				DATE		APPLICATION NO.	DATE
wo						WO 1994-US2397	19940310
	V: AU,						
	RW: AT,	BE,	CH, DE	, DK, ES,	FR,	GB, GR, IE, IT, LU,	MC, NL, PT, SE
CA	2157594		AA	19940915		CA 1994-2157594	19940310
AU	9463974		A1	19940926		CA 1994-2157594 AU 1994-63974	19940310
AU	692766		B2	19980618			
						EP 1994-911470	19940310
EP				19980819			
							LU, MC, NL, PT, SE
JP	08507527		Т2	19960813		JP 1994-520212	19940310
AT	169930		E	19980915		AT 1994-911470	19940310
ES	2123133		Т3	19990101		AT 1994-911470 ES 1994-911470 US 1994-290826 CA 1994-2185123	19940310
US	5637691		Α	19970610		US 1994-290826	19940818
CA	2185123		AA	19950914		CA 1994-2185123	19940913
WO	9524415		A1	19950914		WO 1994-US10265	19940913
	W: AU,	CA,	JP, US				
						GB, GR, IE, IT, LU,	
AU	9480101		A1	19950925		AU 1994-80101	19940913
				19981224			
EP	749437		A1	19961227		EP 1994-931274	19940913
EP				20011205			
							LU, MC, NL, PT, SE
JP	09509959		T2	19971007		JP 1994-523429	19940913
AT	210144		E	20011215		AT 1994-931274 ES 1994-931274	19940913
E5	2164110		Т3	20020216		ES 1994-931274	19940913
US	5721226		A	19980224		US 1995-478763	19950607
PRIORITY	Y APPLN.	INFO.	. :			US 1993-29018	19930310
-						US 1993-29018 WO 1994-US2397 US 1994-290826 WO 1994-US10265	19940310
						US 1994-290826	19940818
						.0 1334 0310203	13340313
						HS 1995-416883	19950420

W0 1994-US10265 19940913
US 1995-416883 19950420
Title compds. (I, X = cationic hydrophilic side chain having .gtoreq.2
pos. charged amino groups; Y = anionic hydrophilic side chain, the steroid
nucleus includes satd., unsatd., or partially satd. rings and .gtoreq.1
substituent selected from OH, SH, F, alkyl, alkoxy, aminor with the
exception of sqalamine) and related compds., were prepd. Thus,
5.alpha.-cholestan-3-one was reductively aminated with
BOC-NH(CRI2 NH(BC) (CRI2) SHM2 and NABH3CN in MeOH to give 71% of an
.alpha., beta.-mixt. of protected cholestan-3-amines which were
deprotected with CF3COZH in CRC13 to give title compd. II and the
.beta.-isomer. II showed a min. inhibitory concn. of 2-4 .mu.g/mL against

L9 ANSWER 12 OF 14 MARPAT COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 114:43309 MARPAT
TITLE: Preparation of sulfonic acid-substituted aromatic steroids as inhibitors of steroid 5.alpha.-reductase
INVENTOR(S): Holt, Dennis Alan; Metcalf, Brian Walter; Levy, Mark
Alan
PATENT ASSIGNEE(S): SmithXline Beecham Corp., USA
Euc. Pat. Appl., 26 pp.
CODEN: EPYXDW
DOCUMENT TYPE: Patent
LANGUAGE: EPYXDW
FAMILY ACC. NUM. COUNT: 1

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 375347	A1	19900627	EP 1989-313260	19891219
EP 375347	B1	19941221		
R: AT, BE,	CH, DE	ES, FR, GB,	GR, IT, LI, LU, NL	, SE
US 4970205	A	19901113	US 1988-290020	19881223
IL 91968	A1	19941021	IL 1989-91968	19891012
CN 1051181	λ	19910508	CN 1989-108217	19891024
CA 2005215	AA	19900623	CA 1989-2005215	19891212
ZA 8909669	Α	19901128	ZA 1989-9669	19891218
DX 8906451	A	19900624	DK 1989-6451	19891219
ES 2066003	Т3	19950301	ES 1989-313260	19891219
AU 8947005	A1	19900628	AU 1989-47005	19891220
AU 627528	B2	19920827		
JP 02225494	A2	19900907	JP 1989-330927	19891220
AU 9229602	A1	19930121	AU 1992-29602	19921124
NII CEECOL		10050105		

AU 9229602 Al 19930121 AU 1992-29602 19921124
AU 655691 B2 19950105
PRIORITY APPLN. INFO.:

US 1988-290020 1988123
AB Title steroids I [X1, X2, X3 = H, Cl. F, Br. iodo, CF3, alkyl, OH, alkoxy, CN. NO2, N(R1)2, CC2R1, CHO R = (1) .alpha.-H, .alpha.-OH, or .alpha.-OAc, and/or various carbonyl-contp, mono- or divalent radicals, (2) .beta.-acylamino, .beta.-cyano, or .beta.-terazolyl and .alpha.-H, (3) keto, etc.; R1 = H, alkyl) and their salts were prepd. For example, Me estrone underwent a sequence of conversion to its enol triflate, aminocarbonylation using (iso-Pr)2NH, hydrogenation of .DELTA.16, and demethylation of 3-OMe to give 3-hydroxyest-1,3,5(10)-triene-17.beta.-(N,N-diisopropylcarboxamide). Acylation of 3-OH with Me2NC(S)Cl, isomerization, and hydrolysis gave the 3-thiol, which was oxidized by O and KOH in DMF to give K estratrienesulfonate deriv. II. The inhibition const. (Ki) of II for steroid 5.alpha.-reductase from hyperplastic human prostate was 10 M. Ten I are claimed, and prepns. with data are given for addnl. precursors of I.

ANSWER 11 OF 14 MARPAT COPYRIGHT 2003 ACS on STN (Continued) Staphylococcus aureus, vs. 0.5-1 .mu.g/mL for sqalamine.

G13-G1--G24

- 66-1 80-3

= alkyl<(1-4)> = 0 = 206

₹ <sub>626</sub>

G25 G26 G27 MPL: NTE:

= alkyl<(1-3)> = alkyl<(1-10)> (SR G27) = CO2H / OH / CF3 claim 1

substitution is restricted

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ANSWER 12 OF 14 MARPAT COPYRIGHT 2003 ACS on STN = 36
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367-C(0)-G10

- alkylene<(1-12)>
- alkyl\*(1-8)> (SO (1-) OH)
- OH
- claim 8
- also incorporates structure from claim 10
- substitution is restricted

L9 ANSWER 13 OF 14
ACCESSION NUMBER:
117:E:
117:E:
118:9890 MARPAT
112:198890 MARPAT
112:198890 MARPAT
112:198890 MARPAT
112:198890 MARPAT
112:198890 MARPAT
Preparation of estratriene derivatives as steroid
5.alpha.-reductase inhibitors
Holt, Dennis Alan; Levy, Mark Alan; Metcalf, Brian
Walter
PATENT ASSIGNEE(5):
SOURCE:

SOURCE:

DOCUMENT TYPE:
LANGUAGE:
FAMILY ACC. NUM. COUNT:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. APPLICATION NO. DATE KIND DATE 

DX 169787 B1 19950227

RITY APPLM. INFO:: US 1988-198534 19880525

The title compds. (I; X1, X2, X3 = H, halo, CF3, C1-6 alkyl, OH, etc.; A = 0, S; n = 0, 1; R1 = H, C1-8 alkyl; R3 = mono- or divalent radical, e.g., H, alkyl, etc.) (II) useful as steroid S.alpha.-reductase inhibitors, were prepd. E.g., 17.beta.-(diisopropylcarbampyl) estra-1,3,5(10)-triene-3-carboxylic acid(II) was prepd. in many steps from estrone via trifluoromethylsulfonylation, carbamoylation, methoxycarbonylation, and hydrogenation. II in vitro inhibited human steroid S.alpha.-reductase with a Ki of 19 nM. Tablets were formulated contg. I.

L9 ANSWER 14 OF 14 MARPAT COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:
TITLE:
New 7-aryl-substituted 19-norsteroids useful as antiproliferatives, antiestrogens, and/or estrogens, and their preparation, use as medicines, and pharmaceutical compositions
Nique, François; Nedelec, Lucien; Bouton, Marie Madelaine; Philibert, Daniel
ROUSSEL-UCLAF, Fr.
EUR. Pat. Appl., 33 pp.
CODEN: EUR. Pat. Appl., 33 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 280618	A1	19880831	EP 1988-400371	19880218
EP 280618	B1	19920930		
R: AT, BE,	CH, DE	ES, FR, GB,	GR, IT, LI, LU, NL	. SE
FR 2610933	A1	19880819	FR 1987-2072	19870218
FR 2610933	B1	19890609		
ZA 8801030	Α	19890426	ZA 1988-1030	19880215
FI 8800742	A	19880819	FI 1988-742	19880217
FI 92589	В	19940831		
AU 8811785	A1	19880825	AU 1988-11785	19880217
AU 610560	B2	19910523		
US 4874754	A	19891017	US 1988-157417	19880217
CA 1313653	A1	19930216	CA 1988-559130	19880217
FI 92589	С	19941212	FI 1988-742	19880217
JP 63222198	A2	19880916	JP 1988-34136	19880218
AT 81133	E	19921015	AT 1988-400371	19880218
ES 2043862	Т3	19940101	ES 1988-400371	19880218
IORITY APPLN. INFO.	:		FR 1987-2072	19870218
			EP 1988-400371	19880218

FR 1987-2072 19870218

19-Norsteroids I [A ring = Al, A2; R = Me, Et; Rl = acyl, alkoxy,
(un)protected OH; R2 = H, (un)substituted C.gtoreq. 8 alkyl, alkenyl, or
alkynyl, C.gtoreq.15 aryl or aralkyl; R1R2 = OCOCH2CH2, OCOCH:CH, O(CH2)3,
OCH2CH:CH; Ar = (un)substituted 5- or 6-membered aryl) are prepd. for use
as antiproliferatives, antiestrogens, and/or estrogens. A soln. of
4-BrH9GGHOCH2CH2NNe2 in THF was treated with CuCl and then with
17. beta.-acetoxyestra-4,6-dien-3-one at -35.degree. to give I (A = Al, R =
Me, R1 = OAc, R2 = H, Ar = .alpha.- and .beta.-GGHOCH2CH2NNe2-4;
.beta./.alpha. > 2:11). The 7.alpha.-isomer was aromatized by CuBr2 and
LiBr at 75.degree. in MeCM, and sapond. by KOH in MeCH, to give
[[(dimethylman(no)ethoxy]phenyl]estratrienediol II. The concn. of II
giving 501 inhibition of growth of mammary tumor cells MCF-7 in a fetal
calf serum culture was 0.1 nM.

MOTE 18

PR

L9 ANSWER 13 OF 14 MARPAT COPYRIGHT 2003 ACS on STN (Continued)

= alkylene<(1-12)> = alkyl<(1-8)> (SO (1-) OH) claim 15

ANSWER 14 OF 14 MARPAT COPYRIGHT 2003 ACS on STN (Continued)

= Ak<(-8)> (SO (1-) G5)
= acyl / COPh / alkoxycarbonyl
= OH
and acid- and base-addition salts
claim 1

### => d his

L6

(FILE 'HOME' ENTERED AT 13:06:43 ON 07 OCT 2003)

FILE 'REGISTRY' ENTERED AT 13:06:52 ON 07 OCT 2003
L1 STRUCTURE UPLOADED
L2 6 S L1
L3 STRUCTURE UPLOADED
L4 5 S L3
L5 66 S L3 FULL

FILE 'CAPLUS' ENTERED AT 13:09:38 ON 07 OCT 2003 3 S L5

FILE 'BEILSTEIN' ENTERED AT 13:13:14 ON 07 OCT 2003 L7 4 S L5

FILE 'MARPAT' ENTERED AT 13:15:30 ON 07 OCT 2003 15 S L5 FULL

L8 15 S L5 FULI L9 14 S L8/COM ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

305813-55-2 CAPLUS
19-Norpregna-1,3,5(10),16-tetraene-20-pentanamine, .alpha.,.alpha.dimethyl-3-[(tris(1-methylethyl)silyl]oxy]-, (205)- (9CI) (CA INDEX NAME)

#### Absolute stereochemistry.

305813-56-3 CAPLUS

Acetamide, N-[(65)-1,1-dimethyl-6-[3-[[tris[1-methylethyl]silyl]oxy]estra-1,3,5(10),16-tetraen-17-yl]heptyl]- (9CI) (CA INDEX NAME)

#### Absolute stereochemistry.

305813-58-5 CAPLUS
19-Norpregna-1,3,5(10),6,16-pentaene-20-pentanamine, .alpha.,.alpha.-dimethyl-3-[[tris(1-methylethyl)silyl)oxy]-, (20R)- (9CI) (CA INDEX NAME)

L4 ANSWER 3 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1995:441032 CAPLUS
DOCUMENT NUMBER: 122:291299
Synthesis of 24,24-dihomo-1.alpha.,25-dihydroxyvitamin
D3 AUTHOR(S): Tachibana, Yoji
Res. Cent., Nisshin Flour Milling Co., Ltd., Saitama, 356, Japan
Chemical & Pharmaceutical Bulletin (1994), 42(11), 2349-51
COODEN: CPBTAL, ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English

COUR: CPBTAL; ISSN: 0009-2363

PUBLISHER: Pharmaceutical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOUNCE(s): CASREACT 122:291298

AB An alternative synthesis of 24,24-dihomo-1.alpha.,25-dihydroxyvitamin D3

was achieved starting from stigmasterol or cholenic acid.

IT 146310-89-69

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(synthesis of dihomodihydroxyvitamin D3)

RN 166310-89-6 CAPLUS

CN Pregna-1,3,5,7-tetraene-20-hexanol, 3-(acetyloxy)-.alpha.,.alpha.-dimethyl, acetate, (2DR)- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued) Absolute stereochemistry.

305813-59-6 CAPLUS Acetamide, N-[(6R)-1,1-dimethyl-6-[3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10),6,16-pentaen-17-yl]heptyl]- (9CI) (CA INDEX NAME)

#### Absolute stereochemistry.

REFERENCE COUNT:

10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 14
ACCESSION NUMBER:
DOCUMENT NUMBER:
1993:124882 CAPLUS
118:124882 CAPLUS
118:124882
118:124882
Preparation of active vitamin D3 derivative as cell differentiation inducer
Tachibana, Yoji
Nisshin Flour Milling Co., Ltd., Japan
Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKOKAF

DOCUMENT TYPE:
DATE OF TACHIBANGUAGE:
Japanese

Japanese

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04300865	A2	19921023	JP 1991-89174	19910329
JP 3129758 ORITY APPLN, INFO.	. B2	20010131	JP 1991-89174	19910329

JP 3129758 B 20010131
PRIORITY APPLM. INTO:

CASREACT 118:124882
AB 24,24-Dihomo-1.alpha,25-dihydroxyvitamin D3 (II), showing cell differentiation activity (no data), is prepd. from 24,24-dihomocholesta-5,7-diene-1.alpha,3:bets.25-tiol (I) by photoirradn. and subsequent thermal isomerization. A soln. of I (prepn. given) in EU20-THF was irradiated by UV, concd., and then after addn. of EUGH, the soln. was heated under cellux for I h to give 24% II.

IT 146310-89-69
RL: RCT (Reactant), SPN (Synthetic preparation), PREP (Preparation), RACT (Reactant or reagent)
(prepn. and redn. of)
RN 146310-89-6 CAPLUS
CP Fregna-1,35,7-tetraene-20-hexanol, 3-(acetyloxy)-.alpha.,.alpha.-dimethyl-, acetate, (20R)- (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1992:6827 CAPLUS
116:6827
TITLE: Preparation of cholesta-5,7-diene-1.alpha.,3.beta.,25triol as intermediate for 1.alpha.,25-dihydroxyvitamin

D3
Tachibana, Yoji
Nisshin Flour Milling Co., Ltd., Japan
Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JXXXAF
Fatent
Japanese
1 INVENTOR(S): PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

KIND DATE PATENT NO.

PATENT NO. KIND DATE APPLICATION NO. DATE

JP 03118392 A2 19910520 JP 1989-254837 19890929

JP 2953665 B2 19990927

PRIORITY APPLN. INFO.: JF 1989-254837 19890929

OTHER SOURCE(S): CASREACT 116:6827 MARPAT 116:6827

AB The title compd. (I) is prepd. via oxidn. of 25-hydroxycholesterol by DDQ, protection of 25-OH in resulting 25-hydroxy-cholesta-1,4,6-triene-3-ons II (R = OH), reaction of II (X = protected OH) with AccCMe:CH2 in the order of alc. IV with 4-phenyl-1,2,4-triazoline-3,5-dione, protection of 3-OH in the adduct V, epoxidn. of 1,2-double bond, deprotection of 3-OH, and redn. of the resulting epoxide VI.

IT 137342-87-19

RL: RCT (Reactant), SPN (Synthetic preparation), PREP (Preparation), RACT (Reactant or reagent) (prepn. and redn. of)

[RN 137342-87-1 CAPLUS]

CN Cholesta-1,3,5,7-tetraene-3,25-diol, diacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

(Continued) L4 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

L4 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER:
109873745 CAPLUS
26,27-Diethyl-1.alpha.,25-dihydroxyvitamin D3 and
24,24-difluoro-24-homo-1.alpha.,25-dihydroxyvitamin
D3: highly potent inducer for differentiation of human
leukemia cells HL-60

AUTHOR(S):

AUTHOR(S):

Lekawa, Nobuoo Eguchi, Tadashi, Hara, Noriyuki,
Takatsuto, Suguru Honda, Atsushi, Mori, Yo, Otomo,
Susumu

CORPORATE SOURCE:

CORPORATE SOURCE:

COBEN: CPBTAL, ISSN: 0009-2363

DOCUMENT TYPE:
LANGUAGE:

COMEN: CPBTAL, ISSN: 0009-2363

DOCUMENT TYPE:
LANGUAGE:

CASREACT 109:73745

AB 26,27-Diethyl-1.alpha.,25-dihydroxyvitamin D3 {I] and 24,24-difluoro-24-homo-1.alpha.,25-dihydroxyvitamin D3 (II) were synthesized. They had
almost no vitamin D activity but were more active than
1.alpha.,25-dihydroxyvitamin D3 in tests for induction of cell
differentiation.

(Insph.,25-dihydroxyvitamin D3 in tests for induction of cell
differentiation.

(prepn. of, during synthesis of vitamin D3 analogs)

RN 115540-34-6 CAPLUS

CN Pregna-4, 6-diene-1,3-diol, 20-(4-hydroxy-4-propylheptyl)-, 1,3-diacetate,
(1.alpha.,3-beta.,208)- (9CI) (CA INDEX NAME)

115540-40-4 CAPLUS Pregna-4,6-diene-1,3-dio1, 20-[5-(acetyloxy)-4,4-difluoro-5-methylhexyl]-, diacetate, (1.alpha.,3.beta.,20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ACCESSION NUMBER:

DOCUMENT NUMBER:

1985:471584 CAPLUS

103:71584

Synthesis of 1.alpha.,25-dihydroxy-26,27-dimethylvitamin D3, a highly active analog of 1.alpha.,25-dihydroxyvitamin D3

AUTHOR(S):

Sai, Hiroshin Takatsuto, Sugurus Hara, Noriyukis Itekswa, Nobuo

CORPORATE SOURCE:

Dep. Chem., Tokyo Inst. Technol., Tokyo, 152, Japan Chemical & Pharmaceutical Bulletin (1985), 33(2), 878-81

COURCET TYPE:

LANGUAGE:

OTHER SOURCE(S):

AB Title vitamin D3 deriv. I was prept. from epoxy(tetrahydropyranyloxy)dinor choladianone II and was more active than 1.alpha.,25-dihydroxyvitamin D3. Key transformations in the prepn. of I included Wittig condensation of norcholenal III (R = MeOCH2) with Ph3P:CHCOZEt and subsequent hydrospenation, Grignadt reaction with EtBr, and hydrolysis to give the tettiary alc. IV (R = H).

Packstart or (reactin) SNN (Synthetic preparation), PREP (Preparation), RACT

97453-13-99 (Reactant), SPN (Synthetic preparation), PREP (Preparation), RACT (Reactant or reagent) (prepn. and sapon. of) 97453-13-9 CAPUS Pregna-4,6-diene-1,3-diol, 20-(4-ethyl-4-hydroxyhexyl)-, 1,3-diacetate, (l.alpha.,3.beta.,20R)- (9CI) (CA INDEX NAME)

09/926,491 Page 10

L4 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER:
103:71583 CAPLUS
103:71583

A stereoselective synthesis of 1,2-diols from
.alpha.-hydroxyaldehydes

AUTHOR(S):
Dolence, E. Kutt; Adamczyk, Maciej; Watt, David S.;
Russell, Graeme B.; Horn, Dennis H. S.
CORPORATE SOURCE:
Dep. Chem., Univ. Wyoning, Laramie, WY, 82071, USA
Tetrahedron Letters (1985), 26(9), 1189-92
CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE:
LANGUAGE:
CASREACT 103:71583

AB The addn. of LiC.tplbond.CCMe20-THP (THP = tetrahydro-2H-pyran-2-yl) to
(20R)-20-hydroxypregnane-20-carboxaldehydes I and II in the absence and in
the presence of BF3 afforded predominantly 20R,22R-diols III and IV or
20R,22S-diols V and VI, resp., characteristic of ecdysones.

IT 97452-03-0P 97452-04-1P
RL: NCT (Reactant): SFN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or respent)
(prepn. and hydrolysis-hydrogenation of)
RN 97452-03-0 CAPUS
CN 19-Norcholesta-1,3,5(10)-trien-23-yne-20,22-diol, 3-methoxy-25[(tetrahydro-2H-pyran-2-yl)oxy]-, (22R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

97452-84-1 CAPLUS
19-Norcholesta-1,3,5(10)-trien-23-yne-20,22-diol, 3-methoxy-25[(tetrahydro-ZH-pyran-2-y1)oxy]-, (225)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

L4 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

97452-85-2P 97452-86-3P
RL: SPN (Synthetic preparation), PREP (Preparation)
(prepn. of)
97452-85-2 CAPLUS
19-Norcholesta-1,3,5(10)-triene-22,25-diol, 3-methoxy-, (22R)- (9CI) (CA INDEX NAME)

97452-86-3 CAPLUS 19-Norcholesta-1,3,5(10)-triene-20,22,25-triol, 3-methoxy-, (22S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1985:62515 CAPLUS
102:62515
An improved synthesis of 1.alpha.-hydroxy-7dehydrocholesterol derivatives
Nishikawa, Osamu, Oshida, Junichi, Tsuruta, Hideki
Pharm. Dev. Sect., Teijin Ltd., Iwakuni, 740, Japan
Chemical 6 Pharmaceutical Bulletin (1984), 32(8),
3244-7

Japan

3244-7

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The effect of protective groups on the allylic bromination and the subsequent dehydrobromination of cholesterol and 1.alpha.hydroxycholesterol derivs. I (R = Ac, Me3CCD, Me(CH2)4CO, EtOZC, PhCH2OZC, R1 = H, AcO, Me3CCO2, Me(CH2)4CO, PhCH2OZC, R3 = H, H0] was examd. 1.alpha.-Hydroxy-7-dehydrocholesterol derivs. were selectively obtained in high yield by using alkoxycarbonyl groups as protective groups.

T7 79488-37-2P

RL: SPN (Synthatic processed)

79488-37-2P
RL: SPN (Synthetic preparation), PREP (Preparation)
(prepn. of, by bromination-dehydrobromination of cholestenol deriv.)
79488-37-2 CAPUS
Cholesta-4, 6-diene-1, 3, 25-triol, 1, 3-bis(ethyl carbonate),
(1.alpha., 3.beta.) - (9CI) (CA INDEX NAME)

L4 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1984:22905 CAPLUS
DOCUMENT NUMBER: 100:22905 Cholecalciferol derivatives
INVENTOR(5): 5 Earner, Richard, Hubscher, Josef
Hoffmann-La Roche, Fr., und Co. A.-G., USA
U.S., 7 pp. Cont.-in-part of U.S. Ser. No. 333,354,
abandomed.
COUDEN: USXXXMM Patent
LANGUAGE: Equipment of U.S. Ser. No. 2003,354,
COUDEN: USXXXMM Patent
LANGUAGE: Equipment of U.S. Ser. No. 333,354,
COUDEN: USXXXMM Patent
Equipment of U.S. Ser. No. 333,354,
COUDEN: USXXXMM Patent
LANGUAGE: Equipment of U.S. Ser. No. 333,354,
COUDEN: USXXXMM Patent OF U.S. Ser. No. 333,354,
COUDEN: USXXMM PATENT OF U.S. SER. NO. 333,354,
COUDENT OF U.S. SER

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE US 4407754 CH 644100 GB 2114569 GB 2114569 PRIORITY APPLN. INFO.: 19831004 19840713 19830824 19840523 A A A1 B2 US 1982-357438 CH 1979-8346 GB 1983-4071 19820312 19790914 19830214 Un 2114569 B2 19840523

IORITY APPLN. INFO.:

US 1980-183140 19800902

US 1981-333354 19811222

GB 1980-29544 198009012

Trihydroxyprecholecalciferol I was prepd. from pregnenecarboxaldehydes II (R, R1 = alkyl, acyl) via Wittig condensation with dioxolanylethylphosphonium salts III (R2, R3 = alkyl, R4 = aryl).

Isomerizing I gave 1.alpha.,25,26-trihydroxycholecalciferol, useful for regulating Ca metab. or Ca transport in mammals (no data):
88257-25-4P

RE: RCT (Reactant), SPN (Synthetic assertion)

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

RE: Restant or reagent

(Restant or reagent

(prepn. and hydrogenation of)

8257-23-4 CAPLUS

Cholesta-4,22-diene-1,3,25,26-tetrol, 1,3-diacetate, (1.alpha.,3.beta.)
(9C1) (CA NOEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

ΙT 88257-30-1P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and ring cleavage of)

L4 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1982:6958 CAPLUS
DOCUMENT NUMBER: 96:6958
1.alpha.-Hydroxy-7-dehydro steroids
Klausmeier, William H., Johnson, Richard L., Hirsch, Arnold L.
PATENT ASSIGNEE(S): Diamond Shamrock Corp., USA
U.S., 9 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
English
FAMILY ACC. NUM. COUNT: 1

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

US 4287129 A 19810901 US 1980-172925 19800728
EP 45894 A1 19820217 EP 1981-105846 19810723
R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE
PRIORITY APPLM. INFO.: US 1980-172925 19800728
AB Unsacd. steroids I (R = cholestane side-chain substituted by HO, AcO, cholane side-chain substituted by AcO, R = alkyl) were preped. as intermediates in the prepn. of vitamin DJ derivs. Thus, oxidn. of 25-hydroxycholesterol by dichlorodicyanobenzoquinone gave 58% 25-hydroxycholesta-1,4,6-trien-3-one, which undervent benzoylation and then enolization-acetylation by treatment with AcO-AcCl in the presence of pyridine to give 3-acetoxy-25-benzoyloxycholesta-1,3,5,7-tetraene. Th latter undervent successive Diels-Alder reaction with 4-phenyl-1,2,4-triazoline-3,5-dione, silylation, and epoxidn. to give epoxycholestene adduct II, which undervent desilylation and LiAlH4 redn. to give 1.alpha. 25-dihydroxy-7-dehydrocholesterol.

80097-53-6P
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)
(prepn. and redn. of)
80097-53-6 CAPLUS
Cholesta-1,3,5,7-tetraene-3,25-diol, 3-acetate 25-benzoate (9CI) (CA INDEX NAME)

ANSWER 10 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued) 88257-30-1 CAPLUS Cholesta-4,7-diene-1,3,25,26-tetrol, (1.alpha.,3.beta.)- (9CI) (CA INDEX NAME)

L4 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1981:569604 CAPLUS
DOCUMENT NUMBER: 95:169604 CAPLUS
1TITLE: 95:169604 CAPLUS
1NVENTOR(S): Active-type vitamin 03 compounds and the cholesta-5, 7-diene precursors
Nishikawa, Osamu; Ishimaru, Kenji; Takeshita, Toru;
Tauruta, Hideki
Teijin Ltd. , Japan
Euc. Pat. Appl., 53 pp.
CODEN: EPKKDW
Patent DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM, COUNT: PATENT INFORMATION: Patent English

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 28484	A1	19810513	EP 1980-303732	19801022
EP 28484			BL 1300 303132	13001022
		, IT, NL, SI		
JP 56059737		19810523		19791023
JP 61045999	B4	19861011		
JP 56092267			JP 1979-169464	19791227
JP 60034948	B4	19850812		
JP 56092268	A2	19810725	JP 1979-169465	19791227
JP 62051266	B4	19871029		
JP 56147765	A2	19811116	JP 1980-50258	19800418
JP 60034949	B4	19850812		
DK 8004473	A	19810424	DK 1980-4473	19801022
DK 160817		19910422		
DK 160817	С	19911007		
CA 1160217	A1	19840110	CA 1980-362937	19801022
US 4388243	A	19830614	US 1982-371870	19820426
PRIORITY APPLN. I	NFO.:		JP 1979-135871	
			JP 1979-169464	19791227
			JP 1979-169465	19791227
			JP 1980~50258	
			US 1980-199126	19801022

US 1980-199126 19801022

Cholestadienes I (R, R1 = alkoxycarbonyl: R2 = H, alkoxycarbonyloxy, R3 = H, alkoxycarbonyloxy, H0) were prepd. as intermediates in the prepn. of 1.alpha.-hydroxycholecalciferol. Thus, treatment of 1.alpha.-hydroxycholesterol wth ClCOZEt in CRICCI2 conts. 4- (dimethylamino)pyridine gave 1.alpha., 3.beta.-bis(ethoxycarbonyloxy)cholest-5-ene, which underwent photochem. bromination by dibromodimethylhydantoin in hexane and then dehydrobromination in xylene contg. collidine at 170.degree. to give I (R = R1 = ECOZC; R2 = R3 = H).

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

(preps. of) 61319-29-7 CAPUS Cholesta-4,6-diene-1,3,25-triol, triacetate, (1.alpha.,3.beta.)- (9CI) (CA INDEX NAME)

09/926,491 Page 12

L4 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

79488-37-2 CAPLUS Cholesta-4,6-diene-1,3,25-triol, 1,3-bis(ethyl carbonate), (1.alpha.,3.beta.)- (9CI) (CA INDEX NAME)

#### Absolute stereochemistry.

L4 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

67804-88+0 CAPLUS

Cholesta-4,6-diene-1,3,25-triol, (l.alpha.,3.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1978:559786 CAPLUS
DOCUMENT NUMBER: 89:159786
TITLE: Determination of 1.alpha.,25-dihydroxycholecalciferol
INVENTOR(S): Baggiolini, Enrico: Uskokovic, Milan Radoje, Fairney,
Angela
PATENT ASSIGNEE(S): Hoffmann-La Roche, F. und Co. A.-G., Fed. Rep. Ger.
SOURCE: COEN: GMOXEX
DOCUMENT TYPE: ALANGUAGE: Patent
LANGUAGE: Patent
LANGUAGE: GERMAN DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. DATE KIND APPLICATION NO. DATE DE 2800782 GB 1592170 DX 7800078 NL 7800224 JP 53087344 FR 2376863 FR 2376863 DX 8001254 PRIORITY APPLN. INFO.: 19780713 19810701 19780708 19780711 19780801 19780804 19800801 19800321 DE 1978-2800782 GB 1977-538 DK 1978-78 NL 1978-224 JP 1978-314 FR 1978-414 19780109 19770107 19780106 19780106 A1 A A A A2 A1 B1 A

Al 19780804 FR 1978-414 19780109

FR 2376863 B1 19800801 DK 1980-1254 19800321

DK 8001254 A 19800321 DK 1980-1254 19800321

DRITY APPLN. INFO.:

GB 1977-538 19770107

DK 1978-78 1978-1010

Antigens and antiserums are prepd. and a radioimmunoassay (RIA) is described for detn. of 1.alpha., 25-dihydroxycholecalciferol(I) and its optical enantiomers and racemates. As antigen, 1.alpha., 25-dihydroxycholecalciferol(25-hemisuccinate (II), which was prepd. by a series of reactions starting with I, was coupled to bovine serum albumin. The II-serum albumin conjugate, in complete Freund's adjuvant, was injected into rabbits to elicit antibody prodn. I in human blood serum then was detd. by RIA that uses the anti-conjugate antiserum, 1-3H as tracer, and dextran-coated charcoal to sep. free from bound antigen. The RIA is sensitive to pg amts. of I. 67804-87-99 67804-88-09

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, dihydroxycholecalciferol radioimmunoassay in relation to) 67804-87-9 CAPLUS

Cholesta-4,6-diene-1,3,25-triol, 1,3-diacetate, (1.alpha.,3.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1977:16846 CAPLUS
B6:16846 CAPLUS
86:16846 CAPLUS
11TILE: 1.alpha.,25-Dihydroxycholecalciferol
1.alpha.,25-Dihydroxycholecalci

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO. DATE	
DE 2607322	A1	19760902	DE 1976-2607322 19760223	
DE 2607322	C2	19830601		
US 3993675	A	19761123	US 1975-552027 19750224	
CH 622533	Α	19810415	CH 1976-1173 19760130	
JP 51108050	A2	19760925	JP 1976-17160 19760220	
JP 59001278	B4	19840111		
BE 838823	A1	19760823	BE 1976-164533 19760223	
FR 2301503	A1	19760917	FR 1976-4939 19760223	
FR 2301503	B1	19800229		
GB 1539061	Α	19790124	GB 1976-7028 19760223	
GB 1539062	Α	19790124	GB 1976-41939 19760223	
AT 351187	В	19790710	AT 1976-1267 19760223	
AT 7601267	Α	19781215		
NL 7601872	Α	19760826	NL 1976-1872 19760224	
NL 173172	В	19830718		
NL 173172	С	19831216		
JP 58116457	A2	19830711	JP 1982-215630 19821210	
JP 59012666	B4	19840324		
RITY APPLN. INFO.	:		US 1975-552027 19750224	
			GB 1976-7028 19760223	
	DE 2607322 DE 2607322 DE 2607322 US 3993675 CH 622533 JP 51108050 JP 59001278 BE 838822 FR 2301503 FR 2301503 FR 2301503 FR 2301503 FR 1539061 GB 1539061 GB 1539061 MI 7501267 MI 73172 ML 773172 ML 773172 JP 58116457 JP 58012666	DE 2607322 A1 DE 2607322 C2 US 3993675 A GE 622533 A JF 51108050 A2 JF 59001278 B4 BE 838823 A1 FR 2301503 B1 GB 1539061 A GB 1539062 A AT 351187 B AT 7601267 A LT 7601872 A LT 7501872 B LL 173172 C JF 58116457 A2	DE 2607322 A1 19760902 DE 2607322 C2 19830601 US 3993675 A 19761123 CH 622533 A 19810415 P 51108050 A2 19760925 JF 59001278 B4 1984011 DE 838823 A1 19760823 PR 2301503 A1 19760827 PR 2301503 A1 19760827 PR 2301503 A1 19760827 PR 2301503 A1 19760917 PR 2301503 A1 19760917 A2 3750124 A3 19790124 A4 7 351187 B 19790710 A4 7 3501267 A 1979124 A4 7 351187 B 19830718 A4 7 351267 A5 19780127 A5 19830718 A5 19830718 A5 19830718 A5 19830711 A5 19830718 A5 19830711 A5 19840324	DE 2607322 A1 19760902 DE 1976-2607322 19760223 DE 2607322 C2 19830601 US 3993675 A 19761123 US 1975-552027 19750224 CH 622533 A 19810415 CH 1976-1173 19760130 JP 51108050 A2 19760925 JP 1976-11716 19760220 JP 59001278 B4 19840111 BE 83823 A1 19760917 FR 1976-4939 19760223 FR 2301503 A1 19760917 FR 1976-4939 19760223 FR 2301503 A1 19760917 GR 1976-4039 19760223 GB 1539061 A 19790124 GB 1976-7028 19760223 GB 1539062 A 19790124 GB 1976-41939 19760223 AT 7601267 A 19780124 GB 1976-1267 19760223 AT 7601267 A 19780126 NI 1976-1267 19760223 AT 7601267 A 19781215 NL 7601872 A 19760826 NL 1976-1872 19760224 NL 173172 B 19831216 NL 173172 C 19831216 NL 173172 C 19831216 JP 58016457 A2 19830711 JP 1982-215630 19821210 JP 58016457 A2 19830711 JP 1982-215630 19821210 JP 58016457 A2 19830711 JP 1982-215630 19821210

Us 1975-35/027 19750224

1.alpha.,25-Dihydroxycholecalciferol (I, R = H) was prepd. by irradn. of 3.beta.-hydroxy-1.alpha.,25-diacetoxycholesta-5,7-diene (II), sapon. of precholecalciferol III (R = Ac), and isomerization of III (R = H). Bromination-dehydrobromination of 1.alpha.,25-diacetoxycholesteryl acetate followed by sapon. gave II.
61319-29-7P
RI: SPN (Synthetic preparation), PREP (Preparation) (prepn. and hydrolysis-dehydration of)
61319-29-7 CAPLUS
CAPLUS (CA INDEX NAME)

L4 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

IT 61319-30-0P
RL: SPN (Synthetic preparation), PREP (Preparation)
(preph. of)
RN 61319-30-0 CAPLUS
CN Cholesta-2,4,6-triene-1,3,25-triol, triacetate, (l.alpha.)- (9CI) (CA INDEX NAME)

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(FILE 'HOME' ENTERED AT 07:50:11 ON 08 OCT 2003)

FILE 'REGISTRY' ENTERED AT 07:50:58 ON 08 OCT 2003 STRUCTURE UPLOADED

L1 STRUCTURE UPLOA L2 0 S L1

L3 83 S L1 FULL

FILE 'CAPLUS' ENTERED AT 07:53:38 ON 08 OCT 2003

L4 14 S L3

L5 14 S L3/PREP L6 0 S L5 NOT L4 => d ibib ab hitstr 1-14

L4 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2003:265913 CAPLUS
DOCUMENT NUMBER: 139:7056
TITLE: Regio- and Stereoselective Ruthenium-Catalyzed
Hydrovinylation of 1,3-Dienes: Application to the
Generation of a 20(5) Stercidal Side Chain
He, Zhengjie: Yi, Chae S., Donaldson, William A.
Department of Chemistry, Marquette University,
Milvaukee, Wi, 5201-1881, USA
Organic Letters (2003), 5(9), 1567-1569
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
JOCUMENT TYPE:
LANGUAGE: English
The addn. of ethylene to 1,3-dienes and 1-vinylcycloalkenes, catalyzed by
two ruthenium complexes, proceeds in a regioselective fashion to afford
3-methyl-1,4-dienes as products. For example, cyclobesene I (R = H,
CMe:CR2, R1 = CH:CR2) gives I (R1 = CHMedCi:CR2) in 57-625 yield. For a
steroidal-based 1-vinylcycloalkene II, the addn. is stereospecific, giving
a product with a 20(5) configuration.

IT 533925-77-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(regio- and stereoselective ruthenium-catalyzed hydrovinylation of
1,2-dienes, vinylcycloalkenes, and steroidal diene)
RN 533925-77-8 CAPIUS
CN 4-Octen-3-ol, 3-ethyl-7-(3-(phenylmethoxy) estra-1,3,5(10),16-tetraen-17y1]-, (4E,75)- (9C1) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

REFERENCE COUNT:

11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued) study, unclassified), RCT (Reactant), SPN (Synthetic preparation), THU (Therapeutic use), BIOL (Biological study), PREP (Preparation), RACT (Reactant or reagent), USES (Uses) (synthesis of cholestane compds. with a c17-alkyl side chain and an arom. A-ring for use in cell modulating therapy) 305812-17-3 CAPLUS Acetamide, N=[68]-6-(3-hydroxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

305812-18-4 CAPLUS 19-Norpregna-1,3,5(10),16-tetraen-3-ol, 20-[5-(ethylamino)-5-methylhexyl]-, (20R)- (9CI) (CA INDEX NAME)

305812-52-6 CAPLUS 19-Norcholesta-1,3,5(10)-trien-23-yne-3,25-diol (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:814500 CAPLUS
DOCUMENT NUMBER: 133:350395
TITLE: Synthesis of cholestane compounds with a c17-alkyl side chain and an aromatic A-ring for use in cell modulating therapy
INVENTOR(S): Hesse, Robert Henry, Setty, Sundara Katugam Srinivasasetty, Ramgopal, Malathi; Kugabalusooriar, Sanna

Sanga Maraden, John, Christopher, UX; Research Institute for Medicine and Chemistry Inc. PCT Int. Appl., 75 pp. CODEN: PIXXIO2 PATENT ASSIGNEE(S):

SOURCE:

DOCUMENT TYPE:

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: English

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		W:	ΑE,	AG,	AL,	AM,	AT,	ΑT,	AU,	AZ,	, в	A,	BB,	BG,	BR,	BY,	CA,	CH,	CN,
																ES,			
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																MN,			
			ΝZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	, s	I,	SK,	SK,	SL,	TJ,	TM,	TR,	TT,
					UĢ,	US,	UΖ,	VN,	YU,	ZA,	, z	w,	ΑM,	ΑZ,	BY,	KG,	ΚŻ,	MD,	RU,
			TJ,	TM															
		RW:	GH,	GM,	ΚĔ,	LS,	MW,	SD,	SL,	SZ,	, т	z,	UG,	Z₩,	AT,	BE,	CH,	CY,	DE,
			DK.	ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	, L	u,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,
			CG,	CI,	CM,	GΑ,	GΝ,	GW,	ML,	MR,	, N	E,	SN,	TD,	TG				
	EP	1179	005		A	1	2002	0213		1	ξP	200	00-9	2756	9	2000	0511		
		R:	AT,	BE,	CH,	DE,	DX,	ES,	FR,	GB,	, G	R,	IT,	LI,	LU,	NL,	SE,	MC,	PT.
							FI,												
																2001			
																2001			
PRIC	RIT	' APP	LN.	INFO	. :					GB 1	199	19-1	1093	4	Α	1999	0511		
										WO 2	200	10-0	B18	13	W	2000	0511		
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Synthesis of cholestane compds. (1) [R1 and R2, which may be the same or different, - alkyl, alkenyl, alkynyl; R3 - Me having, alpha. - or .beta.-configuration; R4 - H or an etherifying or esterifying group; R5 - H, OH, alkowy; X - OM, wherein R4 is as defined above, or NR6R7 wherein R6 - H, aliph, or araliph, org. group, acyl group comprising aliph., araliph, or aryl org. group linked to the nitrogen atom by way of a carbonyl group; R7 - H, alkyl; Y - (un)substituted alkylene, alkenylene, alkynylene; dotted lines signify that double bonds may be present at the 16(17)-position and/or either at the 6(7) - and 8(9)-positions or at the 7(8)-position is disclosed for modulation of cell growth and differentiation, while having low calcemic activity. Thus, I [R1,R2 - Me; R3 - .alpha.-Me; R4,R5 - H; X - NRAc; Y - (CH2)4; .DELTA.16 double bond] is prepd. by reaction of 3-triisopropylsilyloxy-19-norchol-1, 3,5(10),16-tetraene-24-bromide with acetoniltrile followed by redn. of nitrile to amine, mathylation of amine with Me lithium, acetylation of the amino with acetic anhydride and desilylation with TBAF.
305812-17-39 305812-18-49 305812-92-6P
RL: RAC (Biological activity or effector, except adverse); BSU (Biological

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

305812-19-5P 305812-20-8P 305812-21-9P 305812-22-0P 305812-22-0P 305812-23-1P 305812-24-2P 305812-25-3P 305812-26-4P 305812-26-9P 305812-30-0P 305812-31-1P 305812-32-2P 305812-30-0P 305812-31-1P 305812-33-5P 305812-33-3P 305812-34-4P 305812-31-35-9P 305812-36-6P 305812-37-1P 305812-31-39-9P 305812-31-9P 305812-41-3P 305812-42-4P 305812-42-4P 305812-42-4P 305812-41-3P 305812-42-5P 305812-43-5P 305812-43-5P 305812-51-5P 305812-51-5P 305812-51-5P 305812-51-6P 305812-51-6P 305812-51-6P 305812-51-7P 305812-51-9P 305812-51-9P 305812-51-9P 305812-51-9P 305812-51-0P 305812-51-P 30581

Absolute stereochemistry.

305912-20-8 CAPLUS
19-Norpregna-1,3,5(10),16-tetraen-3-o1, 20-[5-(dimethylamino)-5-methylhewyl]-, (20R)- [9CI) (CA INDEX NAME)

ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

305812-21-9 CAPLUS 19-Norpregna-1,35(10),16-tetraen-3-ol, 20-[5-(ethylmethylamino)-5-methylhenyl]-, (20N)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305812-22-0 CAPLUS Acetamide, N-[(6R)-6-(3-methoxyestra-1,3,5(10),16-tetraen-17-y1)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305812-23-1 CAPLUS Acatamide, N-[(6R)-6-(3-ethoxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

Absolute stereochemistry.

305812-27-5 CAPLUS Acetamide, N-[(6R)-6-[(17.beta.)-3-hydroxyestra-1,3,5(10)-trien-17-y1]-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305812-28-6 CAFLUS 19,26,27-Trinorcholesta-1,3,5(10)-triene-3,24-diol, 24-(2-propynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305812-29-7 CAPLUS 19,26,27-Trinorcholesta-1,3,5(10)-triene-3,24-diol, 2-methoxy-24-(2-propynyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

305812-24-2 CAPLUS Acetamide, N-(-(6K)-1,1-dimethyl-6-(3-(2-methylpropoxy)estra-1,3,5(10),16-tetraen-17-yl|heptyl|- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305812-25-3 CAPLUS
Benzamide, N-(16N)-6-(3-hydroxyestra-1,3,5(10),16-tetraen-17-y1)-1,1-dimethylheptyl|- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

305812-26-4 CAPLUS
Benzeneacetamide, N-[(6R)-6-(3-hydroxyestra-1,3,5(10),16-tetraen-17-y1)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN Absolute stereochemistry. (Continued)

Absolute stereochemistry.

305812-30-0 CAPLUS
19,26,27-Trinorcholesta-1,3,5(10)-triene-3,24-diol, 24-(2-propynyl)-,
(205)- (9C1) (CA INDEX NAME)

305812-31-1 CAPLUS

3030312-31-1 CAPBUS
19-Norpregna-1,3,5(10)-trien-3-01, 20-[3-hydroxy-3-(2-propynyl)-1-hexen-5-ynyl]-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

305812-32-2 CAPLUS 19-Norpregna-1,3,5(10)-trien-3-o1, 20-[3-hydroxy-3-(2-propynyl)-1-hexen-5-

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued) ynyl]-2-methoxy-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

RN 305812-33-3 CAPLUS CN 19-Norpregna-1,3,5(10)-trien-3-01, 20-[3-hydroxy-3-(2-propyny1)-1-hexen-5-yny1]-, (205)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

RN 305812-34-4 CAPLUS
CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethyl-2-hexynyl)-, (20R)(9C1) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
CN 19-Norpregna-1,3,5(10)-trien-3-o1, 20-(4-amino-4-ethylhekyl)-, (20R)(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-38-8 CAPLUS
CN 19-Norpregna-1,3,5(10)-trien-3-o1, 20-(4-amino-4-ethylhexyl)-2-methoxy-, (20R)- (9C1) (C1 NNDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c} \text{Me} & \text{(CH2) 3} \\ \text{Me} & \text{R} \\ \text{H} \\ \text{S} & \text{H} \\ \text{H} \\ \text{S} & \text{H} \end{array}$$

RN 305812-39-9 CAPLUS
CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethylhexyl)-, (205)-(9C1) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-40-2 CAPLUS
CN Acetamide, N-[(5R)-1,1-diethyl-5-[(17.beta.)-3-hydroxyestra-1,3,5(10)-trien-17-yl]-2-hexpyyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 305812-35-5 CAPLUS
CN 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethyl-2-hexynyl)-2-methoxy-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-36-6 CAPLUS CN 19-Morpregna-1,3,5(10)-trien-3-o1, 20-(4-amino-4-ethyl-2-hexynyl)-, (20S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-37-7 CAPLUS

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued Absolute stereochemistry.

RN 305812-41-3 CAPLUS
CN Acetamide, M-[(SR)-1,1-diethyl-5-[(17.beta.)-3-hydroxy-2-methoxyestra1,3,5(10)-trien-17-yl]-2-hexynyl]- (SC1) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-42-4 CAPLUS
CN Acetamide, N-[(55)-1,1-diethyl-5-((17.beta.)-3-hydroxyestra-1,3,5(10)-trien-17-yl]-2-hexynyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-43-5 CAPLUS
CN 19-Norpregna-1,3,5(10)-triene-20-methanol, .alpha.-(3-amino-3-ethyl-1-pentynyl)-3-hydroxy-, (203)- (9C1) (CA INDEX NAME)

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued) Absolute stereochemistry.

RN 305812-44-6 CAPLUS
CN 19-Norpregna-1,3,5(10)-triene-20-methanol, .alpha.-(3-amino-3-ethyl-1-pentynyl)-3-hydroxy-2-methoxy-, (205)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-45-7 CAPLUS
CN 19-Norpregna-1,3,5(10)-triene-20-methanol, .alpha.-(3-amino-3-ethyl-1-pentynyl)-3-hydroxy-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued y1)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-49-1 CAPLUS
N 19,26,27-Trinorergosta-1,3,5(10),16-tetraen-3-ol, 24-amino-2-methoxy-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-50-4 CAPLUS
CN Acetanida, N-[(6R)-6-(3-hydcoxyestra-1,3,5,7,9,16-hexaen-17-y1)-1,1dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-51-5 CAPLUS CN 19-Norpregna-1,3,5,7,9,16-hexaen-3-ol, 20-(5-amino-5-methylhexyl)-, (20R)-(9CI) (CA INDEX NAME) L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

RN 305812-46-8 CAPLUS
CN Acetamide, N-[(GR)-6-(3-hydroxy-2-methoxyestra-1,3,5(10),16-tetraen-17-yl)1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-47-9 CAPLUS
CN 19-Norpregna-1,3,5(10),16-tetraen-3-o1, 20-(5-amino-5-methylhexyl)-2-methoxy-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-48-0 CAPLUS
CN Acetamide, N-(3-hydroxy-2-methoxy-19-norcholesta-1,3,5(10),16-tetraen-25-

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued Absolute stereochemistry.

RN 305812-53-7 CAPLUS CN 19-Norcholesta-1,3,5(10)-triene-3,25-diol (9CI) (CA INDEX NAME)

RN 305812-54-8 CAPLUS CN 19-Norcholesta-1,3,5(10)-trien-23-yne-3,25-diol, 2-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-55-9 CAPLUS
CN 19-Norcholesta-1,3,5(10)-trien-23-yne-3,25-diol, (205)- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

305812-56-0 CAPLUS
19-Norcholesta-1,3,5(10)-triene-3,25-diol, 2-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305812-57-1 CAPLUS 19-Norcholesta-1,3,5(10)-triene-3,25-diol, 2-methoxy-, (20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305812-58-2 CAPLUS
19-Norpregna-1,3,5(10)-trien-3-ol, 20-(5-hydroxy-5-methyl-1,3-hexadienyl)-, (20R)- (9CI) (CA INDEX NAME)

ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued) 19-Norcholesta-1,3,5(10),16-tetraen-3-ol, 25-amino-, (205) - (9CI) (CA INDEX NAME)

305812-62-8 CAPLUS Acetamide, N-[(205)-3-hydroxy-19-norcholesta-1,3,5(10),16-tetraen-25-y1]-(9CI) (CA INDEX NAME)

305812-63-9 CAPLUS Acetamide, N-[(6R)-6-(3-hydroxyestra-1,3,5(10),6,16-pentaen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305912-64-0 CAPLUS 19-Norpregna-1,3,5(10),6,16-pentaen-3-ol, 20-(5-amino-5-methylhexyl)-, (20R)- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN Absolute stereochemistry. Double bond geometry unknown.

305812-59-3 CAPLUS 19-Norpregna-1,3,5(10),16-tetraen-3-ol, 20-(5-amino-5-methylhexyl)-, (205)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

305812-60-6 CAPLUS Acetamide, Nr. [(65)-6-(3-hydroxyestra-1,3,5(10),16-tetraen-17-y1)-1,1-dimethylheptyl- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-61-7 CAPLUS

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN Absolute stereochemistry. (Continued)

305813-30-3P 305813-32-5P 305813-36-9P 305813-43-8P 305813-43-8P 305813-43-8P 305813-44-6P 305813-43-8P 305813-44-P 305813-57-9 305813-51-8P 305813-55-2P 305813-55-2P 305813-55-3P 305813-55-3P 305813-56-3P 305813-56-3P 305813-56-3P 305813-56-3P 305813-56-3P 305813-56-3P 305813-56-3P 305813-56-3P 305813-59-6P 305813-59-6P 305813-59-6P 305813-59-6P 305813-30-3P 305813-3P 305813-30-3P 305813-30-3P 305813-30-3P 305813-3P 305813-3P 305813-3P 305813-3P 305813-3P 305813-3P 305813-3P 305813-3P 305813-3

J9-Norpregna-1,3,5(10),16-tetraene-20-pentanamine, .alpha.,.alpha.dimethyl-3-[[tris(1-methylethyl)silyl]oxy]-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305813-32-5 CAPLUS Acetamide, N-[(6R)-1,1-dimethyl-6-[3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10),16-tetraen-17-yl]heptyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN

305813-36-9 CAPLUS
19-Norpregna-1,3,5(10)-triene-20-pentanamine, .alpha.,.alpha.-dimethyl-3-{\tris(1-methylethyl)silyl}oxy}-, (2OR)- (9CI) (CA INDEX NAME)

305813-38-1 CAPLUS Acetamide, N-[(6R)-1,1-dimethyl-6-[(17.beta.)-3-[[tris(1-methylathyl)silyl]oxy]estra-1,3,5(10)-trien-17-yl]heptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305813-41-6 CAPLUS 19.26,77-Trinorcholesta-1,3,5(10)-trien-24-01, 24-(2-propyny1)-3-[[tris(1-methylethyl)sily1)oxy]- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

305813-46-1 CAPLUS
19-Norpregna-1,3,5(10),16-tetraene-20-pentanamine, 2-methoxy.alpha.,alpha.-dimethyl-3-[[tris(1-methylethyl)silyl]oxy]-, (20R)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

305813-47-2 CAPLUS Acetamide, N-[(6R)-6-[2-methoxy-3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10),16-tetraen-17-yl]-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

305813-49-4 CAPLUS
19-Norpregna-1,3,5,7,9,16-hexaene-20-pentanamine, .alpha.,.alpha.-dimethyl-3-[[tris(1-methyl=thyl)silyl]oxy]-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued) Absolute stereochemistry.

305813-43-8 CAPLUS 5-00ten-1-yn-4-ol, 4-(2-propynyl)-7-[(17.beta.)-3-[(tris(1-methylethyl)silyl]oxy]estra-1,3,5(10)-trien-17-yl]-, (7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

305813-44-9 CAPLUS
19-Norpregna-1,3,5(10)-triene-20-methanol, .alpha.-(3-amino-3-ethyl-1-pentynyl)-3-[[trie(1-methylethyl)silyl]oxy]-, (205)- (901) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

305813-50-7 CAPLUS
Acetamide, N-[(6R)-1,1-dimethyl-6-[3-[[tris(1-methylethyl)silyl]oxy]estra1,3,5,7,9,16-hexaen-17-yl]heptyl]- (9CI) (CA INDEX NAME)

305813-51-8 CAPLUS Silane, [[25-((triethylsily1)oxy]-19-norcholesta-1,3,5(10)-trien-23-yn-3-yl]oxy]tris(1-methylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305813-53-0 CAPLUS
3,5-Octadien-2-ol, 2-methyl-7-[(17.beta.)-3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10)-trien-17-yl]-, (7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

L4 ANSWER 1 OF 6
ACCESSION NUMBER:
DOCUMENT NUMBER:
133:350395
171TLE:
Synthesis of cholestane compounds with a c17-alkyl side chain and an acromatic A-ring for use in cell modulating therapy
Herse, Robert Henry: Setty, Sundara Katugam Srinivasasetty Ramgopal, Malathi; Kugabalusocriar, Sanga
PATENT ASSIGNEE(S):
Maraden, John, Christopher, UK; Research Institute for Medicine and Chemistry Inc.
DOCUMENT TYPE:
DOCUMENT TYPE:
DOCUMENT TYPE:
Patent
LANGUAGE:
English FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

WO 2000068246 Al 20001116 WO 2000-6B1813 20000511

W: As, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, C2, CZ, DE, DE, DK, OK, DM, DZ, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, HD, MG, HK, MN, HW, MX, ND, NZ, FL, FT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TH, TZ, UA, UG, US, UZ, VN, YU, ZA, ZV, AM, AZ, BY, KG, KZ, MD, RU, TJ, TH

RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZV, AT, BE, CH, CY, DE, CG, CI, CM, GA, GN, GW, ML, MR, NR, SN, TD, TG

EP 1179005 Al 2020213 EP 2000-927569 20000511

R: AT, BE, CH, DE, DK, BS, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

NO 2001005520 A 20020109 NO 2001-5520 20011112

PRIORITY APPLIAL INFO: GB 1999-10914 A 19990511

WO 2000-GB1813 W 20000511

R: AT, BE, CH. DE, DK, BS, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IT, SI, LT, LY, FI, RO

NO 2001005520 A 20020109 NO 2001-5520 20011112

RITY APPLN. INFO::

SR SOURCE(S):

MARPAT 133:350395

Synthesis of cholestane compds. (1) [Rl and R2, which may be the same or different, = alkyl, alkenyl, alkynyl, R3 = Me having alpha. - or beta.-configuration; R4 = H or an etherifying or esterifying group; R5 = H, OH, alkoxy; X = ORA, wherein R4 is as defined above, or NRGR7 wherein R6 = H, aligh. or araliph. org, group, acyl group comprising aligh, araliph or aryl org, group linked to the nitrogen atom by way of a carbonyl group; R7 = H, alkyl; Y = (un) substituted alkylene, alkynylene; dotted lines signify that double bonds may be present at the 16(17)-position and/or either at the 6(7)- and 8(9)-positions or at the 7(8)-position) is disclosed for modulation of cell growth and differentiation, while having low calcemic activity. Thus, I [R1, R2 = Me; R3 = .alpha.-Me; R4, R5 = H; X = NHAc; Y = (CH2)41. DELTA.16 double bond its prepd. by reaction of 3-triisporpolysilyloxy-19-norchol-1, 3,5(10) flogical amine, methylation of amine with Me lithium, acetylation of the ambno fit acetic anhydride and desilylation with TBAF.
305612-17-39 305812-18-49 308812-22-69

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU

(Continued)

ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS

ΙT

305812-19-5F 305812-20-8P 305812-21-9F 305812-22-0F 305812-22-0F 305812-22-0F 305812-22-1P 305812-22-3P 305812-23-3P 305812-23-3P 305812-23-3P 305812-30-3P 305812-31-1P 305812-31-35-3P 305812-31-3P 305812-31-3F 305812-31-4P 305812-31-3F 305812-31-4P 305812-31-3P 305812-41-3P 305812-43-5P 30

305812-64-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SFN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of cholestane compady; with a c17-alkyl side chain and an arom. A-ring for use in cell modulating therapy)
305812-19-5 CAPLUS
19-Norpregna-1,3,5(10),16-tetraen-3-o1, 20-[5-methyl-5-(methylamino)hexyl]-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305812-20-8 CAPLUS 19-Norpregna-1,3,5(10),16-tetraen-3-ol, 20-[5-(dimethylamino)-5-methylhexyl]-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)
(Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)
{synthesis of cholestane compds. with a c17-alkyl side chain and an arom. A-ring for use in cell modulating therapy)
305812-17-3 CAPLUS
Acetamide, N-[(6R)-6-(3-hydroxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305812-18-4 CAPLUS 19-Norpregnd-1,3,5(10),16-tetraen-3-ol, 20-[5-(ethylamino)-5-methylhexyl]-, (20R)- 9CI) (CA INDEX NAME)

Absolute stereochemistry.

305812-52-6 CAPLUS 19-Norcholesta-1,3,5(10)-trien-23-yne-3,25-diol (9CI) (CA INDEX NAME) Absolute stereochemistry.

ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)

305812-21-9 CAPLUS 19-Nopregna-1,3,5(10),16-tetraen-3-ol, 20-(5-(ethylmethylamino)-5-methylhexyl]-, (20%)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305812-22-0 CAPLUS Acetamide, N-[GR)-6-(3-methoxyestra-1,3,5(10),16-tetraen-17-y1)-1,1-dimethylheptyl]- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

## L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS

305812-24-2 CAPLUS Acetamide, N-[(6K)-1,1-dimethyl-6-[3-(2-methylpropoxy)]estra-1,3,5(10),16-tetraen-17-y1|heptyl|- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

305812-25-3 CAPLUS
Benzamide, N-[(6R)-6-(3-hydroxyestra-1,3,5(10),16-tetraen-17-yl)-1,1-dimethylheptyl}- (9CI) (CA INDEX NAME)

### Absolute stereochemistry.

305812-26-4 CAPLUS
Benzeneacetamide, N-[(GR)-6-(3-hydroxyestra-1,3,5(10),16-tetraen-17-yl)1,1-dimethylheptyl]- (9C1) (CA INDEX NAME)

ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued) 305812-29-7 CAPLUS 19,26,27-Trinoccholesta-1,3,5(10)-triene-3,24-diol, 2-methoxy-24-(24) propynyl)- (9CI) (CA INDEX NAME)

305812-30-0 CAPLUS 19,26,27-Trinorcholesta-1,3,5(10)-triene-3,24-fiol, 24-(2-propynyl)-, (205)- (9C1) (CA INDEX NAME)

## Absolute stereochemistry.

305812-31-1 CAPLUS 19-Nopregna-1,3,5(10)-trien,3-ol, 20-(3-hydroxy-3-(2-propynyl)-1-hexen-5-ynyl]-, (20R)- (9c) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)

305812-27-5 CAPLUS Acetamide, N-[(GR)-6-{(17.beta.)-3-hydroxyestra-1,3,5(10)-trien-17-y1}-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305812-28-6 CAPLUS 19,26,27-Trinorcholesta-1,3,5(10)-triene-3,24-diol, 24-(2-propynyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

### ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)

305812-32-2 CAPLUS
19-Norpregna-1,3,5(10)-trien-3-ol, 20-[3-hydroxy-3-(2-propynyl)-1-hexen-5-ynyl]-2-methoxy-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

305812-33-3 CAPLUS
19-Norpregna-1,3,5(10)-trien-3-01, 20-{3-hydroxy-3-{2-propynyl}-1-hexen-5-ynyl}-, (205)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

ANSVER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued) 305812-34-4 CAPLUS 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethyl-2-hexynyl)-, (20R)-(9CI) (CA INDEX NAME)

305812-35-5 CAPLUS 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethyl-2-hexynyl)-2-methoxy-, (20R)- (9CI) (CA INDEX NAME)

305812-36-6 CAPLUS 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethyl-2-hexynyl)-, (20S)-(9C1) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS

305812-40-2 CAPLUS Acetamide, N-[(5R)-1,1-diethyl-5-[(17.beta.)-3-hydroxyestra-1,3,5(10)-trien-17-yl]-2-hexynyl]- (9CI) (CA INDEX NAME)

305812-41-3 CAPLUS Acetamide, N-[(5R)-1,1-1,3,5(10)-trien-17-y1) .1-diethyl-5-{(17.beta.)-3-hydroxy-2-methoxyestra-l]-2-hexynyl]- (9CI) (CA INDEX NAME)

305812-42-4 CAPLUS Acetamide, N-[(5S)-1,1-diethyl-5-[(17.beta.)-3-hydroxyestra-1,3,5(10)-trien-17-yl]-2-hexynyl]- (9Ci) (CA INDEX NAME)

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS

305812-37-7 CAPLUS 19-Norpregna-1,3,5(10)-trien-3-ol,20-(4-amino-4-ethylhexyl)-, (20R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

305812-38-8 CAPLUS 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethylhexyl)-2-methoxy-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305812-39-9 CAPLUS 19-Norpregna-1,3,5(10)-trien-3-ol, 20-(4-amino-4-ethylhexyl)-, (205)-(9C1) (CA INDEX NAME)

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued) Absolute stereochemistry.

305812-43-5 CAPLUS 19-Norpregna-1,3,5(10)-triene-20-methanol, .alpha.-(3-amino-3-ethyl-1-pentynyl)-3-hydroxy-, (205)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305812-44-6 CAPLUS 19-Norprgnan-1, 1,5(10)-triene-20-methanol, .alpha.-(3-amino-3-ethyl-1-pentynyl)-3-hydroxy-2-methoxy-, (205)- (SCI) (CA INDEX NAME)

Absolute stereochemistry.

305812-45-7 CAPLUS 19-Norpregna-1,3,5(10)-triene-20-methanol, .alpha.-(3-amino-3-ethyl-1-

ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued) pentynyl)-3-hydroxy-, (20R)- (9CI) (CA INDEX NAME)

305812-46-8 CAPLUS Acetamide, N-[(6R)-6-(3-hydroxy-2-methoxyestra-1,3,5(10),16-tetraen-17-y1)-1,1-dimethylhepty1)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305812-47-9 CAPLUS 19-Norpregna-1,3,5(10),16-tetraen-3-ol, 20-{5-amino-5-methylhexyl}-2-methoxy-, (20R)- {9CI} (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS

305812-54-8 CAPLUS 19-Norcholesta-1,3,5(10)-trien-23-yne-3,25-diol, 2-methoxy- (9CI) (CA INDEX NAME)

305812-55-9 CAPLUS 19-Norcholesta-1,3,5(10)-trien-23-yne-3,25-diol, (205)- (9CI) (CA INDEX NAME)

Absolute stereochemi

305912-56-0 CAPLUS 19-Norcholesta-1,3,5(10)-triene-3,25-diol, 2-methoxy- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS

305812-48-0 CAPLUS Acetamide, N-(3-hydroxy-2-methoxy-19-norcholests-1,3,5(10),16-tetraen-25-y1)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 305812-49-1 CAPLUS
CN 19.26,27-Trinorprosta-1,3,5(10),16-tetraen-3-ol, 24-amino-2-methoxy-(9CI) (CA INDEX NAME)
Absolute stereoghemistry.

RN 305812-53-7 CAPLUS CN 19-Norcholesta-1,3,5(10)-triene-3,25-diol (9CI) (CA INDEX NAME) Absolute stereochemistry.

ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)

305812-57-1 CAPLUS
19-Norcholesta-1,3,5(10)-triene-3,25-diol, 2-methoxy-, (205)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305812-58-2 CAPLUS 19-Morpregns-1,3,5(10)-trien-3-ol, 20-(5-hydroxy-5-methyl-1,3-hexadienyl)-, (20R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

305812-59-3 CAPULS 19-Norpregnen-1,3,5(10),16-tetraen-3-ol, 20-(5-amino-5-methylhexyl)-, (205)- (9C1) (CA INDEX NAME)

## L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)

305812-60-6 CAPLUS Acetamide, N-[(65)-6-(3-hydroxyestra-1,3,5(10),16-tetraen-17-y1)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

305812-61-7 CAPLUS 19-Norcholesta-1,3,5(10),16-tetraen-3-ol, 25-amino-, (20S)- (9CI) (CA INDEX NAME)

### Absolute stereochemistry.

305812-62-8 CAPLUS Acctamide, N-[(205)-3-hydroxy-19-norcholesta-1,3,5(10),16-tetraep-25-y1]-(9C1) (CA INDEX NAME)

ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)
305813-51-8F 305813-53-0F 305813-55-2F
305813-56-3F 305813-58-5F 305813-59-6F
RE: RCT (Reactant) > SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of cholestane compds. with a c17-flkyl side chain and an arom. A-ring for use in cell modulating therapy)
305813-30-3 CAPLUS
19-Norpregna-1,3,5(10),16-tetraene-20-pentanamine, .alpha.,alpha.-dimethyl-3-[{tris(1-methylethyl)silyl]oxy}- (20R)- (9CI) (CA INDEX NAME)

305813-32-5 CAPLUS Acetamide, N-[(68)-1,1-dimethyl-6-[3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10),16-tetraen-17-ylheptyl]- (9C1) (CA INDEX NAME)

## Absolute stereochemistry.

ng CAPLUS gna-1,3,5(10)-triene-20-pentanamine, .alpha.,.alpha.-dimethyl-3-methylethyl)silyljoxy]-, (20R)- (9CI) (CA INDEX NAME) 305813-36-6 19-Norpress [[tris(1/me

## eochemistry.

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued) Absolute stereochemistry.

305812-63-9 CAPLUS Acetamide, N-[(6R)-6-(3-hydroxyestra-1,3,5(10),6,16-pentaen-17-yl)-1,1-dimethylheptyl]- (9CI) (CA INDEX NAME)

## Absolute stereochemistry

305812-64-0 CAPLUS
19-Norpregna-1,3,5(10),6,16-pentaen-3-ol, 20-(5-amino-5-methylhexyl)-, (20R)-(9CI) (CA INDEX NAME)

### Absolute stereochemistry.

305813-30-3P 305813-32-5P 305813-36-9P 305813-3B-1P 305813-41-6P 305813-43-8P 305813-44-9P 305813-46-1P 305813-47-2P

## ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)

305813-38-1 CAPLUS Acetamide, N-[(6R)-1,1-dimethyl-6-[(17.beta.)-3-[[tris(1-methylethyl)silyl]oxy]estra-1,3,5(10)-trien-17-yl]heptyl]- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

305813-41-6 CAPLUS
19.26,27-Trinorcholesta-1,3,5(10)-trien-24-01, 24-(2-propynyl)-3-([tris(1-methylethyl)sizyl)oxy)-(9CI) (CA INDEX NAME)

## Absolute stereochemistry.

305813-43-8 CAPLUS 5-OCTEAN-1-yn-4-01, 4-{2-propynyl}-7-[(17.beta.)-3-[[tris(1-methylethyl) silyl]oxy]estra-1,3,5(10)-trien-17-yl]-, (7R)- (9CI) (CA INDEX NAME)

(Continued)

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued) Double bond geometry unknown.

305813-44-9 CAPLUS 19-Norpregna-1,3,5(10)-triene-20-methanol, .alpha.-(3-amino-3-ethyl-1-pentynyl)-3-{{tris(1-methylethyl)silyl]oxy}-, (20\$)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305813-46-1 CAPLUS
19-Norpregna-1,3,5(10),16-tetraene-20-pentanamine, 2-methoxyalpha.,alpha.-dimethyl-3-[[tris(1-methylethyl)silyl]oxy]-, (20R)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry. Double bond geometry unknown.

Absolute stereochemistry.

305813-56-3 CAPI Acetamide, N-[(65]-1,1-dimethyl-6-[3-[{tris(1-methylethyl)silyl]oxy}estra-1,3,5(10),16-tetfaen-17-yl]heptyl]- (9CI) (CA INDEX NAME)

Absolute stereocher

30,813-58-5 CAPLUS
19-Norpregna-1,3,5(10),6,16-pentaene-20-pentanamine, .alpha.,.alpha.,dimethyl-3-{{tris(1-methylethyl)silyl}oxy}-, (20R)- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS

305813-47-2 CAPLUS
Acetamide, N-[(6R)-6-[2-methoxy,3-[{tris(1-methylethyl)silyl]oxy]estra1,3,5(10),16-tetraen-17-yl]-1,d-dimethylheptyl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

305gf3-51-8 CAPLUS Sylane, [[25-([triethylsily1)oxy]-19-norcholesta-1,3,5(10)-trien-23-yn-3-yl]loxyltris(1-methyl)ethyl)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

305813-53-0 CAPIUS
3,5-Octadien-2-ol, 2-methyl-7-[(17.beta.)-3-{{tris(1-methylethyl)silyl]oxy}estra-1,3,5(10)-trien-17-yl}-, (7R)- (9CI) (CA

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)

Absolute stereochemistry.

 $\label{eq:capus_section} 305813-59-6 \quad \text{CAPLUS} \\ \text{Acetamide, N-[(6R)-1,1-dimethyl-6-[3-[[tris(1-methylethyl)silyl]oxy]estral,3,5(10),6,16-pentaen-17-yl]heptyl]- (9CI) \quad (CA INDEX NAME)}$ 

Absolute stereochemistry.

REFERENCE COUNT: THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1993:64626 CAPLUS
DOCUMENT NUMBER: 132:2029
TITLE: Studies on the constituents of Cyclanthera pedata fruits: isolation and structure elucidation of new triterpenoid saponins
DE Tommasi, Numziatina, De Simone, Francesco, Speranza, Giovanna; Pizza, Cosimo
Dipartimento di Science Farmaceutiche Facolta di Farmacia, Universita di Salerno, Fisciano, 84084, Italy
SOURCE: Journal of Agricultural and Food Chemistry (1999), 47(11), 4512-4519
CODEN: JAFCAU, ISSN: 0021-8561
ADELISHER: American Chemical Society
DOCUMENT TYPE: Journal
ABD The isolation of nine triterpenoid saponins, among them six new natural compds., from the MeOH ext. of the fruits of Cyclanthera pedata is reported. All of the structures were elucidated by spectroscopic methods, including the concerted application of ons-dimensional IH-IH total correlation spectroscopy, IH-IH nuclear Overhauser effect spectroscopy, and 13C-13C DEPT-NNR and two-dimensional MNR techniques (double-quantum filtered correlated spectroscopy, crating-frame Overhauser enhancement spectroscopy, heteronuclear single quantum coherence, and heteronuclear multiple bond correlation). A comparative study of seeds and fruits has been also carried out.

IT 25102-64-4
RL: BOC (Biological study) OCCU (Occurrence);

Absolute stereochemistry. Currently available stereo shown.

L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1994:73386 CAPLUS
DOCUMENT NUMBER: 1294:73386 CAPLUS
TITLE: New nor- and hepta nor-cucurbitacin glucosides from Fevillea trilobata
AUTHOR(S): Valente, Ligia M. H., Gunatilaka, A. A. Leslie; Glass, Thomas E., Kingston, David G. I.; Pinto, Angelo C.
Dep. Chem., Virginia Folytech. Inst. and State Univ., Blacksburg, VA, 24061-0212, USA
Journal of Natural Products (1993), 56(10), 1772-8
CODEN: JNPRDF; ISSN: 0163-3864
Journal
AB From the MeOH ext. of the seeds of Fevillea trilobata (Cucurbitaceae) were isolated fevicordin A glucoside (1), cayaponoside B, cayaponoside D, a new norcucurbitacin glucoside, and a new heptanorcucurbitacin glucoside (1), was established as 29-nor-1, 2, 3, 4, 5, 10-dehydro-2-0--beta.-D-glucopyanosyl-3, 16.alpha., 20R, 22. xi. - tetrahydroxy-1-concucurbitacin B glucoside, and 22, 23, 24, 25, 26, 27, 29-heptanor-1, 2, 3, 4, 5, 10-dehydro-2-0-beta.-D-glucopyanosyl-3, 16.alpha., 20R, 22. xi. - tetrahydroxy-1-chedydro-2-0-beta.-D-glucopyanosyl-3, 16.alpha.-dihydroxycucurbita-11, 20-dione.
RL: BIOL (Biological study)
(from Fevillea trilobata)
RN 152340-777-7 CAPLUS

Absolute stereochemistry.

Absolute stereochemistry.

Absolute stereochemistry. Double bond geometry as shown.

ANSWER 2 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)

THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT REFERENCE COUNT: 16

L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS ACCESSION NUMBER: 1994:73357 CAPLUS DOCUMENT NUMBER: 120:73357 TITLE: Constituents of tropic 120:73357
Constituents of tropical medicinal plants. 59.
Constituents of Fevillea cordifolia: new
norcucurbitacin and cucurbitacin glycosides
Achenbach, Hans; Waibel, Reiner; Hefter-Buebl, Ursula;
Constenla, Manuel A.
Inst. Phacm. Food Chem., Univ. Erlangen, Erlangen,
D-91052, Germany
Journal of Natural Products (1993), 56(9), 1506-19
CODEN: JNRRDF; ISSN: 0163-3864 AUTHOR(S): CORPORATE SOURCE: JOURNAL OR NATURAL PRODUCTS (1993), 56(9), 1506-19 CODEN: JNRDE; ISSN: 0163-3864

MENT TYPE: JOURNAL JOURNAL PRODUCTS: DOUBLE SENSING OF STREET STREE DOCUMENT TYPE:

Absolute stereochemistry. Double bond geometry as

152340-33-5 CAPLUS 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 2,3,16,20,25-pentahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)

152340-34-6 CAPLUS 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 2,3,16,20,25-pentahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,238)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

152340-35-7 CAPLUS

192-Norcholesta-1,3,5(10),23-tetraen-11-one, 2,3,16,20,22,25-hexahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,225,23E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued) Absolute stereochemistry. Double bond geometry as shown.

152340-09-5, Fevicordin B
RL: PROC (Process)
(structure and isolation of, from Fevillea cordifolia seeds)
152340-09-5 CAPLUS
19-Norcholesta-1,3,5(10)-triene-11,22-dione, 25-(acetyloxy)-2,3,16,20-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)

IT

111250-02-3, Fevicordin A RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(Uses) (From Fevilles cordifolia, antinflammatory activity of)
11250-02-3 CAPLUS
19-Norcholasta-1,3,5(10),23-tetraene-11,22-dione, 25-(acetyloxy)-2,3,16,20-tetrahydroxy-4,3,14-trimethyl-, (3.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

ΙT

151589-29-6P, 2,3-Di-O-methylfevicordin A
RL: SPN (Synthetic preparation); PREP (Preparation)
(preph. of)
151589-29-6 CAPLUS
19-Norcholesta-1,3,5(10),23-tetraene-11,22-dione, 25-(acetyloxy)-16,20-dihydroxy-2,3-dimethoxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI)
(CA INDEX NAME)

SOURCE:

L4 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1987:617953 CAPLUS
DOCUMENT NUMBER: 107:217953
TITLE: Fevicordin A and fevicordin A glucoside, novel
norcucurbitacins from Fevilles cordifolia
ACHENDAD, Hansy Hefter-Buebl, Ursulay Constenla,
Manuel A.
Loss Parm Univ. Krlangen-Nuernberg, Erlangen.

Manuel A.
Inst. Pharm., Univ. Erlangen-Nuernberg, Erlangen,
D-8520, Fed. Rep. Ger.
Journal of the Chemical Society, Chemical
Communications (1987), (6), 441-2
CODEN: JCCCAT; ISSN: 0022-4936

CORPORATE SOURCE:

DOCUMENT TYPE: LANGUAGE: AB Fevicordi:

CODEN: JCCCAT; ISSN: 0022-4936

MENT TYPE: JOURNAL

ENGISH
Fevicordin A glucoside and fevicordin A, isolated from the seeds of
Fevillea cordifolia, have structures I (R - .beta.-glucosyl) and I (R H), resp., on the basis of chem. and spectral data.

111250-02-3P, Fevicordin A

RL: PREP (Preparation)
(from Fevillea cordifolia, isolation and mol. structure detn. of)
111250-02-3 CAPLUS
19-Norcholesta-1,3,5(10),23-tetraene-11,22-dione, 25-(acetyloxy)-2,3,16,20-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry. Double bond geometry as shown.

L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER:
1985:471583 CAPLUS
103:71583
A stereoselective synthesis of 1,2-diols from
.alpha.-hydroxyaldehydes
AUTHOR(S):
Dolence, E. Kutt; Adanczyk, Maciej; Watt, David S.;
Russell, Graeme B.; Horn, Dennis H. S.
CORPORATE SOURCE:
Dep. Chem., Univ. Wyoning, Laramie, WY, 82071, USA
SOURCE:
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE:
LANGUAGE:
CASREACT 103:71583
AB The addn. of LiC.tplbond.CCMe20-THP (THP = tetrahydro-2H-pyran-2-yl) to
(20R)-20-hydroxypregnane-20-carboxaldehydes I and II in the absence and in
the presence of BF3 afforded predominantly 20R,22R-diols III and IV or
20R,22S-diols V and VI, resp., characteristic of ecdysones.

IT 97452-83-0P 97452-84-IP
RL: RCT (Reactant): SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and hydrolysis-hydrogenation of)
RN 97452-83-O CAPLUS
CN 19-Norcholesta-1, 3, 5(0) -trien-23-yne-20, 22-diol, 3-methoxy-25[(tetrahydro-22H-pyran-2-yl)oxyl-, (22R)- (9CI) (CA INDEX NAME)
Absolute stereochemistry.

97452-84-1 CAPLUS 19-Norcholesta-1,3,5(10)-trien-23-yne-20,22-diol, 3-methoxy-25-[(tetrahydro-2H-pyran-2-yl)oxy]-, (22S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS (Continued)

97452-85-2P 97452-86-3P
RL: SPN (Synthetic preparation), PREP (Preparation)
(prepn. of)
97452-85-2 CAPLUS
19-Norcholesta-1,3,5(10)-triene-22,25-diol, 3-methoxy-, (22R)- (9CI) (CA INDEX NAME)

97452-86-3 CAPLUS 19-Norcholesta-1,3,5(10)-triene-20,22,25-triol, 3-methoxy-, (22S)- (9CI) (CA INDEX NAME)

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=> file reg

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
29.72 178.29

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE
ENTRY
SESSION
CA SUBSCRIBER PRICE

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-3.91

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Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> d his

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FILE 'REGISTRY' ENTERED AT 12:20:52 ON 03 APR 2003

L1 STRUCTURE UPLOADED

L2 6 S L1

L3 74 S L1 FULL

FILE 'CAPLUS' ENTERED AT 12:21:43 ON 03 APR 2003 L4 6 S L3

FILE 'REGISTRY' ENTERED AT 12:25:15 ON 03 APR 2003

Uploading 491.str

L5 STRUCTURE UPLOADED

=> s 15 sub=13 full FULL SUBSET SEARCH INITIATED 12:25:58 FILE 'REGISTRY' FULL SUBSET SCREEN SEARCH COMPLETED - 74 TO ITERATE

100.0% PROCESSED 74 ITERATIONS SEARCH TIME: 00.00.01

74 ANSWERS

L6 74 SEA SUB=L3 SSS FUL L5

=> del 15- y

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
35.70 213.99

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL
ENTRY SESSION
CA SUBSCRIBER PRICE

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FILE COVERS 1907 - 3 Apr 2003 VOL 138 ISS 14 FILE LAST UPDATED: 2 Apr 2003 (20030402/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

L5 6 L3

=> s 15 not 14

L6 0 L5 NOT L4

=> file beil

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 0.42 214.41 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE 0.00 -3.91

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FILE LAST UPDATED ON MARCH 18, 2003

FILE COVERS 1771 TO 2002.
\*\*\* FILE CONTAINS 8,583,155 SUBSTANCES \*\*\*

>>> PLEASE NOTE: Reaction and substance documents are stored in different file segments. Use separate queries to search for reaction and substance data. When searching for bibliographic information you have the option to chose the file segment. (Use "/XXX.SUB" to search for a bibliographic term in substance documents. To restrict the search to reaction documents use "/XXX.RX".)

For additional information see HELP RXS. <<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

=> s 11 full FULL SEARCH INITIATED 12:26:38 FILE 'BEILSTEIN' FULL SCREEN SEARCH COMPLETED - 924 TO ITERATE

100.0% PROCESSED 924 ITERATIONS SEARCH TIME: 00.00.08

7 ANSWERS

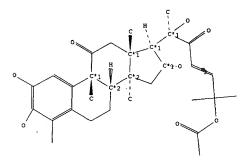
L7 7 SEA SSS FUL L1

=> d all 1-7

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## L7 ANSWER 1 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): Chemical Name (CN): Autonom Name (AUN): 7106735
fevicordin A
acetic acid 5-hydroxy-1,1-dimethyl-4-oxo-5(2,3,16-trihydroxy-4,9,13,14-tetramethyl11-oxo-7,8,9,11,12,13,14,15,16,17decahydro-6H-cyclopenta<a>phenanthren-17yl)-hex-2-enyl ester
C31 H42 08
542.67
10305, 1155
Stereo compound
isocyclic
6159741
6807808
6-08 7106735 Molec. Formula (MF):
Molecular Weight (MW):
Lawson Number (LN):
File Segment (FS):
Compound Type (CTYPE):
Constitution ID (CONSID):
Tautomer ID (TAUTID):
Beilstein Citation (BSO):
Entry Date (DED):
Update Date (DUPD): 6-08 1995/05/11 1995/05/11



- Atom/Bond Notes:
  1. CIP Descriptor: R
  2. CIP Descriptor: S
  3. CIP Descriptor: E

## Field Availability:

Code BBN Beilstein Records

ANSWER 1 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CD5 MDL (Continued) J.Chem.Soc.Chem.Commun., CODEN: JCCCAT(6), <1987>, 441-442; BABS-5938125

```
ANSWER 1 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL
CN Chemical Name 1
AUN Autonomname 1
MP Molecular Formula 1
FW Formular Weight 1
LN Lawson Number 2
File Sagment 1
CTYPE Compound Type 1
CONSID Constitution 1D 1
TAUTID Tautomer ID 1
BSO Beilstein Citation 1
ED Entry Date 1
INP Isolation from Natural Product 1
RSTR Related Structure 1
I AUSTRALL COMPANIAN CO
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     (Continued)
```

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
********		
RX	Reaction Documents	1
RXREA	Substance is Reaction Reactant	1

## Related Structure: RSTR

(RSTR):

The author investigated the configuration

(ASIA):
Reference(s):
1. Achenbach, Hans, Hefter-Buebl, Ursula; Constenla, Manuel A.,
J.Chem.Soc.Chem.Commun., CODEN: JCCCAT(6), <1987>, 441-442;
BABS-5938125

## Isolation from Natural Product: INP

(INP):

Fevillea cordifolia (Cucurbitaceae)

Reference(s):

1. Achenbach, Hans: Hefter-Buebl, Ursula: Constenla, Manuel A.,
J.Chem.Soc.Chem.Commun., CODEN: JCCCAT(6), <1987>, 441-442;
BABS-5938125

## Reaction: RX

Reaction ID (.ID): Reactant BRN (.RBRN): Reactant (.RCT): Product BRN (.PBRN): Product (.PRO): 4023468 7106735 fevicordin A 7103057

/10J057 17-acetyl-2-hydroxy-3-methoxy-4,9,13,14-tetramethyl-6,7,8,9,12,13,14,15-octahydro-cyclopenta<a>phenanthren-11-one

No. of React. Details (.NVAR):

## Reaction Details:

Reaction RID (.RID): 4023468.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): MaBH4, NaIO4, H+/H2O
Reference(s): 1. Achenbach, Hans; Hefter-Buebl, Ursula; Constenla, Manuel A.,

## L7 ANSWER 2 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MOL

Beilstein Records (BRN): CAS Reg. No. (RN): Chemical Name (CN): 4728055 97452-83-0, 97452-84-1

2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<=>phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-

Autonom Name (AUN):

1991/12/02

Gloi 7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta-a>phenanthren-17-y1)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-

diol C32 H46 05 510.71 17122, 6760, 289 Stereo compound Molec. Formula (MF):
Molecular Weight (MW):
Lawson Number (LN):
File Segment (FS):
Compound Type (CTYFE):
Constitution ID (CONSID):
Tautomer ID (TAUTD):
Beilstein Citation (BSO):
Entry Date (DED):
Update Date (DUPD): heterocyclic 4263612 4567456 6-17 1991/12/02

- Atom/Bond Notes:
  1. CIP Descriptor: S
  2. CIP Descriptor: R
- Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records CAS Registry Number	1
CN AUN	Chemical Name	1
MF	Autonomname Molecular Formula	1

09/926,491 Page 15

L7 ANSWER 2 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL (Continued) cyclopenta(a>phenanthren-17-y1)-6-methy1-6-(tetrahydro-pytran-2-y1oxy)-hept-4-yn-e2,3-(Continued) diol 4722039 \*/22U39
2-(3-methoxy-13-methyl7,8,9,11,12,13,14,15,16,17-decahydro-6Hcyclopenta<a>phenanthren-17-yl)-6-methylhept-4-yne-2,3,6-triol Product BRN (.PBRN): Product (.PRO): ED UPD Entry Date Update Date No. of React. Details (.NVAR): Reaction Details: This substance also occurs in Reaction Documents: Reaction RID (.RID): 2742338.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 90 percent (BRN=4722039)
Reagent (.RGT): 70 percent HCIO4
Solvent (.SOL): H2O, methanol Occurrence Code Reaction Documents Substance is Reaction Reactant Substance is Reaction Product RX RXREA RXPRO Reference(s):
1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.;
Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>,
1189-1192; BABS-5554079 Reaction: RX Reaction ID (.ID): Reactant BRN (.RBRN): Reactant (.RCT): 2442472 4525023, 4133964 4525023, 4133964
2-hydroxy-2-(3-methoxy-13-methyl7,8,9,11,12,13,14,15,16,17-decahydro-6Kcyclopenta-aphenanthren-17-y1)
- propionaldehyde, C10H15BrHgO2
4728055, 4728054
2-(3-methoxy-13-methyl7,4,9,11,12,13,14,15,16,17-decahydro-6Hcyclopenta-aphenanthren-17-y1)-6-methyl-6(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3diol, 2-(3-methoxy-13-methyl7,8,9,11,12,13,14,15,16,17-decahydro-6Hcyclopenta-aphenanthren-17-y1)-6-methyl-6(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3diol Reaction: Reaction ID (.ID): Reactant BRN (.RBRN): Reactant (.RCT): 2742337 4728055 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopentaca>phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-Product BRN (.PBRN): Product (.PRO): diol 4722038 Product BRN (.PBRN): Product (.PRO): 4722038 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-17-yl)-6-methyl-hept-4-yne-2,3,6-triol No. of React. Details (.NVAR): No. of React. Details (.NVAR): Reaction Details: Reaction Details: Reaction RID (.RID): 2442472.1
Reaction Classification (.CL): Preparation
Solvent (.SDL): tetrahydrofuran
Temperature (.T): -26 Cel
Note(s) (.COM): Yield given. Yields of byproduct given
Reference(s):
1. Dolence, E. Kurt, Adamczyk, Haciej; Watt, David S., Russell, Graeme B.,
Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>,
1189-1192; BABS-5554079 Reaction RID (.RID): 2742337.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 90 percent (BRN-4722038)
Reagent (.RGT): 70 percent HCLO4
Solvent (.SCL): H2O, methanol
Reference(s): 1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.;
HOrn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>,
1189-1192; BABS-5554079 Reaction: Reaction ID (.ID): Reactant BRN (.RBRN): Reactant (.RCT): 2742338 4728055 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-ANSWER 3 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL L7 ANSWER 3 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL (Continued) Formular Weight Lawson Number File Segment Beilstein Records (BRN): CAS Reg. No. (RN): Chemical Name (CN): 4728054 97452-83-0, 97452-84-1 FS CTYPE 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-Compound Type Constitution ID CONSID TAUTID Tautomer ID Beilstein Citation BSO Entry Date Update Date 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopentaca>phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-Autonom Name (AUN): UPD This substance also occurs in Reaction Documents: dio1 C32 H46 O5 Code Name Molec. Formula (MF):
Molecular Weight (MW):
Lawson Number (LN):
File Segment (FS):
Compound Type (CTYPE):
Constitution ID (CONSID):
Tautomer ID (TAUTID):
Beilatein Citation (BSO):
Entry Date (MED): Occurrence C32 H46 O5 510.71 17122, 6760, 289 Stereo compound heterocyclic 4263612 4567455 RX RXPRO Reaction Documents Substance is Reaction Product Reaction: RX Reaction ID (.ID): Reactant BRN (.RBRN): Reactant (.RCT): 4755023, 4133964
2-hydroxy-2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopentaca>phenanthren-17-yl)-propionaldehyde, [Cl0H15B:HgO2 4728055, 4728054
2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopentaca>phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol, 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopentaca>phenanthren-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-diol 6-17 1991/12/02 1991/12/02 4525023, 4133964 Entry Date (DED): Update Date (DUPD): Product BRN (.PBRN): Product (.PRO): No. of React. Details (.NVAR): Reaction Details: Reaction RID (.RID): 2442472.1
Reaction Classification (.CL): Preparation
Solvent (.SOL): tetrahydrofuran
Temperature (.T): -26 Cel
Note(s) (.COM): Yield given. Yields of byproduct given
Reference(s):
1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.;
Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>,
1189-1192; BABS-5554079

Atom/Bond Notes:
1. CIP Descriptor: S
2. CIP Descriptor: R
Field Availability:

Beilstein Records CAS Registry Number Chemical Name Autonomname Molecular Formula Occurrence

Code

BRN

## ANSWER 4 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): Chemical Name (CN): 4722039
2-(3-methoxy-13-methyl-7,6,5,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-17-yl)-6-methyl-hept-4-yne-2,3,6-triol
2-(3-methoxy-13-methyl-7,8,5,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-17-yl)-6-methyl-hept-4-yne-2,3,6-triol
C27 H38 O4
426.59
6760, 289
Stereo compound
isocyclic
4257630
4557405
6-06 4722039 Autonom Name (AUN): Molec. Formula (MF):
Molecular Weight (NW):
Lawson Number (LN):
File Segment (FS):
Compound Type (CTYPE):
Constitution ID (CONSID):
Tautomer ID (TAUTIO):
Beilstein Citation (BSO):
Entry Date (DED):
Update Date (DUPD): 6-06 1991/12/02 1991/12/02

# Atom/Bond Notes: 1. CIP Descriptor: S 2. CIP Descriptor: R

### Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	i
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1

L7 ANSWER 4 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL (Continued) Reaction Details:

Reaction RID (.RID): 2737115.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): H2
Catalyst (.CAT): Pto2
Reference(s): 1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.;
Horn, Dennis, H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>, 1189-1192; BABS-5554079

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
_=======		
RX	Reaction Documents	:
RXREA	Substance is Reaction Reactant	
RXPRO	Substance is Reaction Product	

## Reaction: RX

Reaction ID (.ID): Reactant BRN (.RBRN): Reactant (.RCT): 2742338 4728055

4/2003 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta(apphenanth(en-17-yl)-6-methyl-6-(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-

diol 4722039

Product BRN (.PBRN): Product (.PRO):

4722039
2-(3-methoxy-13-methyl7,4,9,11,12,13,14,15,16,17-decahydro-6Hcyclopenta<a>phenanthren-17-yl)-6-methylhept-4-yne-2,3,6-triol

No. of React. Details (.NVAR):

## Reaction Details:

Solvent (1301): Reference(9):

1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.; Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>, 1189-1192; BABS-5554079

## Reaction:

Reaction ID (.ID): Reactant BRN (.RBRN): Reactant (.RCT):

2737115
4722039
2-(3-methoxy-13-methyl7,8,9,11,12,13,14,15,16,17-decahydro-6Hcyclopenta<a>phenanthren-17-y1)-6-methylhept-4-yne-2,3,6-triol
471973 4719751
2-(3-methoxy-13-methyl7,8,9,11,12,13,14,15,16,17-decahydro-GHcyclopenta<apheniahrhen-17-yl)-6-methylheptane-2,3,6-triol
1 Product BRN (.PBRN): Product (.PRO):

No. of React. Details (.NVAR):

## L7 ANSWER 5 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): Chemical Name (CN): 4722038

Autonom Name (AUN):

4722038
2-(3-methoxy-13-methyl7,8,9,11,12,13,14,15,16,17-decahydro-6Hcyclopenta<a>phenanthren-17-yl)-6-methylhept-4-yne-2,3,6-triol
2-(3-methoxy-13-methyl7,8,9,11,12,13,14,15,16,17-decahydro-6Hcyclopenta<a>phenanthren-17-yl)-6-methylhept-4-yna-2,3,6-triol
C27 H38 04
26.59
6760, 289
Stereo compound
isocyclic
4257630
4557404 Molec. Formula (MF):
Molecular Weight (MW):
Lawson Number (LN):
File Segment (FS):
Compound Type (CTYPE):
Constitution ID (CONSID):
Tautomer ID (TAUTID):
Beilstein Citation (BSO):
Entry Date (DED):
Update Date (DUPD): 4557404 6-06 1991/12/02 1991/12/02

Atom/Bond Notes: 1. CIP Descriptor: S 2. CIP Descriptor: R

## Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	i

ANSWER 5 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL ED Entry Date 1 Update Date 1 This substance also occurs in Reaction Documents: Reaction Documents Substance is Reaction Reactant Substance is Reaction Product Reaction: RX 2742337
4728055
2-(3-methoxy-13-methyl7,8,9,11,12,13,14,15,16,17-decahydro-6Hcyclopentaca>phenanthren-17-yl)-6-methyl-6(tetrahydro-pyran-2-yloxy)-hept-4-yne-2,3-Reaction ID (.ID): Reactant BRN (.RBRN): Reactant (.RCT): Product BRN (.PBRN): Product (.PRO): 2.2008
2-(3-methoxy-13-methyl7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta
cyclopenta
a>phenanthren-17-yl)-6-methyl-hept-4-yne-2,3,6-triol No. of React. Details (.NVAR): Reaction Details: | Reaction RID (.RID): 2742337.1 |
| Reaction Classification (.CL): Preparation | 90 percent (BRN=4722038) |
| Reagent (.RGT): 70 percent HCIO4 |
| Solvent (.SOL): H2O, methanol Reference(s):

1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.; Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>, 1189-1192; BABS-5554079 Reaction: Reaction ID (.ID): Reactant BRN (.RBRN): Reactant (.RCT): 4722038 4/22/32 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta<a>phenanthren-17-yl)-6-methyl-hept-4-yne-2,3,6-triol 4719750 Product BRN (.PBRN): Product (.PRO): % 17.50
2-(3-methoxy-13-methyl7,8,9,11,12,13,14,15,16,17-decahydro-6Hcyclopenta<a>phenanthren-17-yl)-6-methylheptane-2,3,6-triol

L7 ANSWER 6 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): Beilstein Pref. RN (BPR): CAS Reg. No. (RN): Chemical Name (CN):

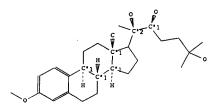
No. of React. Details (.NVAR):

Reaction Details:

Autonom Name (AUN):

HTT 2003 BELISTEIN CDS MOL

4719751
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97452-86 Molec. Formula (MF):
Molecular Weight (MW):
Lawson Number (LN):
File Segment (FS):
Compound Type (CTYPE):
Constitution ID (CONSID):
Tautomer ID (TAUTID):
Beilstein Citation (BSO):
Entry Date (DED):
Update Date (DUPD): 1993/03/20



Atom/Bond Notes:
1. CIP Descriptor: S
2. CIP Descriptor: R

## Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	ī
MF	Molecular Formula	ī
FV	Formular Weight	ī
LN	Lawson Number	2
FS	File Segment	ī

AMSWER 5 OF 7 BELLSTEIN COPYRIGHT 2003 BELLSTEIN CDS MDL (Continued)
Reaction RID (.RID): 2737114.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): H2
Catalyst (.CAT): PtO2
Reference(s):
1. Dolence, E. Kurt; Adamczyk, Haciej; Watt, David S.; Russell, Graeme B.;
Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>,
1189-1192; BABS-5554079

ANSWER 6 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL
CTYPE Compound Type
CONSID Constitution ID 1
TAUTID 1
Tautomer ID 1 (Continued) Compound Type Constitution ID Tautomer ID Beilstein Citation BSO Ed Entry Date Update Date Nuclear Magnetic Resonance

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

Nuclear Magnetic Resonance:

Description (.KW): Nucleus (.NUC): Solvents (.SOL): Chemical shifts pyridine-d5

Solvence (1901): pyrioine-do Reference(s):

1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.; Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>, 1189-1192; BABS-5554079

Reaction: RX

Reaction ID (.ID): Reactant BRN (.RERN): Reactant (.RCT):

4722039 22-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopents<a>phenanthren-17-yl)-6-methyl-hept-4-yne-2,3,6-triol 4719751

Product BRN (.PBRN): Product (.PRO):

4/19/51 2-(3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopentaxa>phenanthren-17-yl)-6-methyl-heptane-2,3,6-triol

No. of React. Details (.NVAR):

Reaction Details:

Reaction RID (.RID): 2737115.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): H2
Catalyst (.CAT): PtO2
Reference(s):
1. Dolence, E. Kurtı Adamczyk, Maciejı Watt, David S.; Russell, Graeme B.;
Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>, 1189-1192; BABS-5554079

## ANSWER 7 OF 7 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

HT 2003 BELISTEIN CDS MDL
4719750
97452-86-3
97452-86-3
97452-86-3
2-(3-methoxy-13-methyl7,6,7,11,12,13,14,15,16,17-decahydro-6Hcyclopenta<apphenanthren-17-yl)-6-methylheptane-2,3,6-triol
2-(3-methoxy-13-methyl7,8,9,11,12,13,14,15,16,17-decahydro-6Hcyclopenta<apphenanthren-17-yl)-6-methylheptane-2,3,6-triol
C27 Ha2 04
430.63
6704, 289
Stereo compound
isocyclic
4257631
4555533
6-06
1991/12/02
1993/03/20 Beilstein Records (BRN): Beilstein Pref. RN (BPR): CAS Reg. No. (RN): Chemical Name (CN): Autonom Name (AUN): Molec. Formula (MF):
Molecular Weight (MW):
Lawson Number (LN):
File Segment (FS):
Compound Type (CTYPE):
Constitution ID (CONSID):
Tautomer ID (TAUTID):
Bellstein Citation (BSO):
Entry Date (DED):
Update Date (DUPD):

Atom/Bond Notes:
1. CIP Descriptor: S
2. CIP Descriptor: R

### Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FV	Formular Weight	1

This substance also occurs in Reaction Documents: Code RX RXPRO Reaction Documents Substance is Reaction Product Nuclear Magnetic Resonance: Description (.KW): Chemical shifts
Nucleus (.NUC): 13C
Solvents (.SOL): pyridine-d5
Reference(s):
1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.;
Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>,
1189-1192; BABS-5554079 Reaction: RX Reaction ID (.ID): Reactant BRN (.RBRN): Reactant (.RCT): 2737114 2737114
4722038
2-(3-methoxy-13-methyl7,8,9,11,12,13,14,15,16,17-decahydro-GHcyclopenta<a>phenanthren-17-yl)-6-methylhept-4-yne-2,3,6-triol
4719750 4719750
2-(3-methoxy-13-methyl7,8,9,11,12,13,14,15,16,17-decahydro-6Hcyclopenta<a>phenanthren-17-yl)-6-methylheptane-2,3,6-triol Product BRN (.PBRN): Product (.PRO): No. of React. Details (.NVAR): Reaction Details: RX Reaction RID (.RID): 2737114.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): H2
Catalyst (.CAT): PtO2
Reference(s):
1. Dolence, E. Kurt; Adamczyk, Maciej; Watt, David S.; Russell, Graeme B.;
Horn, Dennis H. S., Tetrahedron Lett., CODEN: TELEAY, 26(9), <1985>,
1189-1192; BABS-5554079

09/926,491 Page 19

=> d his

(FILE 'HOME' ENTERED AT 12:19:54 ON 03 APR 2003)

FILE 'REGISTRY' ENTERED AT 12:20:52 ON 03 APR 2003

L1 STRUCTURE UPLOADED

L2 6 S L1

L3 74 S L1 FULL

FILE 'CAPLUS' ENTERED AT 12:21:43 ON 03 APR 2003

L4 6 S L3

FILE 'REGISTRY' ENTERED AT 12:25:15 ON 03 APR 2003

FILE 'CAPLUS' ENTERED AT 12:26:14 ON 03 APR 2003

L5 6 S L3

L6 0 S L5 NOT L4

FILE 'BEILSTEIN' ENTERED AT 12:26:28 ON 03 APR 2003

L7 7 S L1 FULL

=> d ibib ab fqhit 1-16

```
L10 ANSWER 1 OF 16 MARPAT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 138:73420 MARPAT
TITLE: Preparation of anti-estrogenic steroids, and
associated pharmaceutical compositions and methods of
                                                                                                                                                                                                                                                                                                                                                                L10 ANSWER 1 OF 16 MARPAT COPYRIGHT 2003 ACS (Continued)
                                                                                                                                                                                                                                                                                                                                                                ትደ-
                                                                                              associated pharmaceutical compositions and method use
Tanabe, Masato, Peters, Richard H., Chao, Van-Ru, Jong, Ling
SRI International, USA
U.S., 50 pr., Cont. of U.S. Ser. No. 220,408.
CODEN: USXXAM
Patent
English
4
    INVENTOR (S):
    PATENT ASSIGNEE(S):
SOURCE:
   DOCUMENT TYPE:
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
                                                                                                                                                                                                                                                                                                                                                                106 647
                       PATENT NO.
                                                                                      KIND
                                                                                                           DATE
                                                                                                                                                                  APPLICATION NO.
                                                                                                                                                                                                                                DATE
                   G43
G45
G47
DER:
MPL:
NTE:
                                                                                                                                                                                                                                                                                                                                                                                        = Ak (SO)

= 0

= alkyl<(1-24)> (SO)

or pharmaceutically acceptable salts or esters

disclosure

oxo substitution also disclosed
   US 6503896
US 6054446
US 6281205
PRIORITY APPLN. INFO.:
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
                                                                                                                                                                                                                                                                                                                                                                REFERENCE COUNT:
  G4
                             - 28
            O ANSWER 2 OF 16 MARPAT COPYRIGHT 2003 ACS
CESSHON NUMBER: 137:370278 MARPAT
TLE: Preparation of substituted pregna-1,3,5(10)-triene
derivatives for pharmaceutical use
Hesse, Robert Henry Setty, Sundara Katugam
Scinivassetty; Prechet, Maurice Murdoch; Gile, Michael
Marsden, John Christopher, UK; Research Institute for
Medicine and Chemistry Inc.
COEN: PIXXD2
Patent
NGUAGE: PIXXD2
Patent
English
MILY ACC. NUM. COUNT: 1
TENT INFORMATION:
                                                                                                                                                                                                                                                                                                                                                                L10 ANSWER 2 OF 16 MARPAT COPYRIGHT 2003 ACS
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             (Continued)
   INVENTOR(S):
   PATENT ASSIGNEE(S):
    SOURCE:
                                                                                                                                                                                                                                                                                                                                                                                        = alkyl<(1-3)>
= NH2
   DOCUMENT TYPE:
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
                                                                                                                                                                                                                                                                                                                                                                                                NM2 claim 1 total carbon content of G8 does not exceed three atoms substitution is restricted
PATENT INFORMATION:

PATENT NO. XIND DATE APPLICATION NO. DATE

WO 2002092100 A1 A0 2021121 NO 2002-GB2210 20020513

W: AE, AG, AL, AM, AT. AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CC, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JF, KR, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, HA, MD, MG, MK, NH, MY, MX, MZ, NO, NZ, CM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, HW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GW, ML, MR, NE, SN, TD, TG
PRIORITY APEIN. INFO:

US 2001-290013P 20010511

AB Pregna-1,3,5(10)-triene derivs., such as I (RI = H, hydroxy protecting group; R2 = OH, CHO, alkowy, alkenyl, alkyl, etc., R3 = .alpha.-, .beta.-Me; X = Cl.-3 alkylene group, bond; Y = CR4) (RS) IMRGF1; R4, N5 = H, alkyl, alkenyl and alkynyl groups, such that the total carbon content of R4 and R5 does not exceed three atoms; R6 = H, aliph. or araliph org, group, acyl, etc.; C16-C17 = satd., unsatd.), were prepd. for a variety of therapeutic uses, such as modulating cell activity, including antiproliferative and antiangiogenic effects. Thus, pregna-1,3,5(10)-triene derivs. II (Y = NHZ, NKCOMe) were prepd via a multistep synthetic series starting from 2-methoxy-3-{[tris(1-methylethyl)silyl]oxy]-estra-1,3,5(10)-triene derivs. III (Y = NHZ, NKCOMe) were prepd via a multistep synthetic series starting from 2-methoxy-3-{[tris(1-methylethyl)silyl]oxy]-estra-1,3,5(10)-triene derivs. IN, NKCOMe) were grepd. Compds. but specific pharmaceutical activity testing data was not presented.
                                                                                                                                                                                                                                                                                                                                                                REFERENCE COUNT:
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
```

(Continued)

```
L10 ANSWER 3 OF 16
ACCESSION NUMBER:
137:47357 MARRAT
TITLE:
INVENTOR(5):
Agoston, Gregory E., Shah, Jamshed H., Hunsucker,
Kimberly A., Pribluda, Victor S., Lavallee, Theresa
M., Green, Shawn J., Herbstritt, Christopher J., Zhan,
Xiaoguo H., Treston, Anthony M.
USA
USA
USA
USA
USA
COODE: USXXCO
DOCUMENT TYPE:
LANGUAGE:
FAMILV ACC. NUM. COUNT:
PATENT INFORMATION:
COUNTY C.
FAMILV ACC. NUM. COUNT:
PATENT INFORMATION:
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  L10 ANSWER 3 OF 16 MARPAT COPYRIGHT 2003 ACS (NTE: additional double bond formation also claim
                                       PATENT NO. KIND DATE APPLICATION NO. DATE

US 2002082433 A1 20020627 US 2001-939208 20010824
RITY APPLN. INFO: US 2000-641327 20000818
US 2000-2533087 2000127
US 2000-2533087 2000127
US 2000-2533087 2000123
US 2001-2782509 2001023
2-Methoxyestradiol derivs. of formula I [R], R4 H, halo, CN, alkyl, OH, NH2, etc., R2 = N3, CN, OMe, alkenyl, alkynyl, alkoxy, NH2, etc., R3 - OH, OAc; R5 - alkyl, alkenyl, dijalkylamino, OH, alkylene, etc., P66, R7 - H, alkyl, alkenyl, alkoyl, alkoyl, alkenyl, alkenyl, alkoyl, Treating mammalian disease characterized by undesirable angiogenesis. Thus, II was prepd. for Treating mammalian from 2-methoxyestradiol and propyltriphenylphosphonium bromide. The IC50 of II against MDA-MB-231 breast tumor cells was 51.31 mu.M.
            US 2002082433
PRIORITY APPLN. INFO.:
                                                                      alkoxy<(-10)> (SO (1-) F
                                       -G13
            ĦĞ-
                                                     - alkyl<(1-10)>
- CF3 / OH
claim 1
                                                                                                                                                        (SO (1-) G21)
         L10 ANSWER 4 OF 16 MARPAT COPYRIGHT 2003 ACS

ACCESSION NUMBER:

I137:6309 MARPAT
Preparation of 2-methoxyestradiol analogs as antiangiogenic agents
Agoston, Gregory: Shah, Jamshed H.; Hunsucker, Kimberly A.; Pribluda, Victor: Lavallee, Theresa M.; Green, Shawn J.; Herbstritt, Christopher J.; Zhan, Xiaoguo H.; Treaton, Anthony

PATENT ASSIGNEE(S):

ENTEMMENT ASSIGNEE(S):

DOCUMENT TYPE:
LANGUAGE:
LANGUAGE:
PIXENT
PATENT INFORMATION:

English
English
FAILY ACC. NUM. COUNT:
PATENT INFORMATION:
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                L10 ANSWER 4 OF 16 MARPAT COPYRIGHT 2003 ACS G8 = 53
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  Ħ2-
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            -G13
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       alkyl<(1-10)> (50 (1-) G21)
CF3 / OM-
claim.1
additional double bond formation also claimed
PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

WO 2002042319 A2 20020530 WO 2001-US26490 20010824

WO 2002042319 A3 20030313

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JF, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PR, PJ, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TH, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RM: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NI, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GM, GG, GW, ML, NR, NE, SN, TD, TG

AU 2001089386 AS 20020603 AU 2001-0823885 20010224

AB 2-Methoxyestradiol analogs, such as I (RI, R3 = H; halo, CM, aikyl, OH, CH2OH, NH2, alkylaminor R2 = N3, CN, C. tplbond.CR, C-CHR, C. tplbond.CH, OR, aminor R = H, alkyl, Z = COH, COAc dashed-bond = single bond or double bond R6 = H, OH, O, oxime, amino, alkyl, alkenyl, R4, R5 = H, alkyl, alkenyl, alkynyl, were prepd for treating mammalian disease characterized by undesirable angiogenesis. Thus, 2-methoxyestradiol analog II was prepd. by the reaction of methyltriphenylphosphonium bromide and 2-methoxyestrone. In vitro evaluation against MDA-MB-231 breast tumor cells and HUVEC endothelial cells, II showed ICSO 0.24.+-.0 and 0.19.+-0.19 resp.
                                                     - alkoxy<(-10)
                                                                                                                                                   (SO (1-) F)
```

```
L10 ANSWER 5 OF 16
ACCESSION NUMBER:
136:232440 MARRAT
TITLE:
Preparation of novel anti-estrogenic steroids
Tanabe, Masator Peters, Richard H.; Chao, Wan-rus
Jong, Ling
USA
SOURCE:
USA
U.S. Pat. Appl. Publ., 56 pp., Cont.-in-part of U.S.
6,281,205.
CODEN: USXXCO
DOCUMENT TYPE:
LANGUAGE:
English
 DOCUMENT TYPE:
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
         US 2002032180
US 6054446
US 6281205
PRIORITY APPLN. INFO.:
```

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L10 ANSWER 6 OF 16
ACCESSION NUMBER:
135:358085 MARPAT
TITLE:
Preparation of 2-substituted pregna-1,3,5(10)-triene
and chola-1,3,5(10)-triene derivatives with
antiproliferative and antiangiogenic activity
Hesse, Robert Henry; Setty, Sundara Katugam
Stinivasasetty; Pechet, Maurice Murdoch; Gile, Michael
Marsden, John Christopher, UK; Research Institute for
Medicine and Chemistry Inc.
PCT Int. Appl., 40 pp.
CODEN: PIXXD2

DOCUMENT TYPE:
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:

135:358085 MARPAT
Preparation of 2-substituted pregna-1,3,5(10)-triene
and chola-1,3,5(10)-triene derivatives with
antiproliferative and antiangiogenic activity
Actually Support Suppor
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DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

WO 2001085755 Al 20011115 WO 2001-082103 20010511

W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, PK, PK, BZ, CA, CH, CN, CO, CR, CU, CZ, CZ, DE, DK, DK, DK, DM, DZ, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LA, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MK, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SI, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, TV, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TH

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, WM, LM, RN, NE, SN, TD, TG

EF 1287017 Al 20030305 EF 2001-928120 /20010511

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NS, EM, CPT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

NO 2002005392 A 2003099 NO 2002-5392 20021111

PRIORITY APPLN. INFO: US 2003-0908 PR 2004-928120 CH2OH, etc.) are preped. which exhibit potent cell modulating activity, including antiproliferative and antiangiogenic effects. Thus, 2-methoxy-3-triangropylsilyloxy-19-norpregn-1,3,5(10),77(20)2-tetraene (prepn. given) is reacted with Me acrylate, reduced with LiAlH4, and desilylated with TBAF to give II.

G3

- 23

L10 ANSWER 5 OF 16 MARPAT COPYRIGHT 2003 ACS `G31 āč--G5 G24 G25 G27 G31 Me Ak (SR (1-) G26) alkyl<(1-24)> MPL: NTE: or pharmaceutically acceptable salts or esters

```
L10 ANSWER 6 OF 16 MARPAT COPYRIGHT 2003 ACS (Continued)
            alkyl<(1-3)>
            claim 1 total carbon content of G8 does not exceed three atoms substitution is restricted
                                          THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
REFERENCE COUNT:
```

L10 ANSWER 7 OF 16 MARPAT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 135:195698 MARPAT
TITLE: Preparation of anti-estrogenic steroids, and
associated pharmaceutical compositions and methods of Use Tanabe, Masato; Peters, Richard H.; Chao, Wan-ru; Jong, Ling Sri International, USA U.S., 50 pp., Cont.-in-part of U.S. 6,054,446. CODEN: USKXAM Patent English 4 INVENTOR(S): PATENT ASSIGNEE(S): SOURCE: DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: PATENT NO. KIND DATE APPLICATION NO. DATE

US 6281205 US 6054446 US 2002032180 US 6503896 US 2002032181 US 6455517 PRIORITY APPLN. INFO.: B1 A A1 B1 A1 B1 20010828 20000425 20020314 20030107 20020314 20020924 US 1998-220408 US 1997-998877 US 2001-872825 US 2001-872826 US 2001-918890 19981224 19971224 20010531

US 6455517 B1 20020924

DRITY APPLN. INFO::

US 1997-998877 19971224

Novel antiestrogenic compds. are prepd. which are useful to treat a variety of disorders, patricularly estrogen-dependent disorders.

Preferred compds. have a 1,3,5(10)-estratiene nucleus, and are .

substituted at the C-17 or C-11 position with a mol. moiety which renders the compds. effective to competitively block the binding of estrogen to its receptor. Particularly preferred compds. are 17-desoxy-1,3,5(10)-estratienes, e.g. of formula I [Rl = H, alkoxy, halo, CN, etc., R2 = H, OH, alkyl, etc., R3 = H, alkyl, acyl, SOZNHZ, etc., R4, R5 = H, alkyl, hetcroyclyl etc., L = (substituted) five- or six-membered cyclic moiety; m = 1-6; p = 0-6). Thus, II citrate salt was prepd. and showed strong growth inhibitory activity against MCF-7 human mammary tumor at 10 mg/kg/day. Therapeutic methods and pharmaceutical compns. are provided as well.

MSTR 1

G3 - 23

LIO ANSWER 8 OF 16
ACCESSION NUMBER:
133:350395 MARPAT
Synthesis of cholestane compounds with a c17-alkyl side chain and an aromatic A-ring for use in cell modulating therapy
INVENTOR(S):
RESERVED AND ANSIGNEE (S):
PATENT ASSIGNEE (S):
SOURCE:
SOURCE:
COURT TYPE:
LANGUAGE:
FAMILY ACC. NUM. COUNT:
FAMILY ACC. NUM. COU

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

NO 2001005520 A 20020109 NO 2001-5520 20011112

Synthesis of cholestane compds. (I) (R1 and R2, which may be the same or different, = alkyl, alkenyl, alkynyl; R3 = Me having, alpha.- or .beta.-configurations R4 = H or an etherifying or esterifying group; R5 = H, OH, alkowy, X = OM, wherein R4 is as defined above, or NR6R7 wherein R6 = H, aliph. or araliph. org. group; nuked to the nitrogen atom by way of a carbonyl group; R7 = H, alkyl; Y = (un)substituted alkylene, alkenylene, alkynylene; dotted lines signify that double bonds may be present at the 16(17)-position and/or either at the 6(7)- and 8(9)-positions or at the 16(17)-position, while having low calcemic activity. Thus, I (R1, R2 - Me; R3 = .alpha.-Me; R4, R5 = H, X = NNAC; Y = (CH2)4; DELTA.16 double bond] is prepd. by reaction of attrisopropylsilyloxy-19-norchol-1,3,5(10),16-tetraene-24-bromide with acetonicitie followed by redn. of nitrile to amine, methylation of amine with Me lithum, acetylation of the amino with acetic anhydride and desilylation with TBAF.

L10 ANSWER 7 OF 16 MARPAT COPYRIGHT 2003 ACS (Continued)

`G31

¥8--G5

= Me = Ak (SR (1-) G26) = 0 = alkyl<(1-24)>

claim 3 or pharmaceutically acceptable salts or esters oxo substitution also claimed also incorporates broader disclosure

REFERENCE COUNT:

THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT 38

L10 ANSWER 8 OF 16 MARPAT COPYRIGHT 2003 ACS (Continued)

G12

loweralkylOH

loweralkylene (SO G10) OH

claim 1

REFERENCE COUNT:

THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L10 ANSWER 9 OF 16 MARPAT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 132:152024 MARPAT
TITLE: Preparation of steroids as inhibitors of type 3
3.alpha.-hydroxysteroid dehydrogenase
Labrie, Fernand, Merand, Yves; Gauthier, Sylvain,
Provencher, Louis; Luu-The, Van
Provencher, Louis; Luu-The, Van
Endorecher, Louis; Luu-The, Van
Provencher, Louis; Luu-The, Van
Endorecher, Louis; Luu-The, Va
            LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
                                                                        PATENT NO.
                                                                                                                                                                                                                                                                                    KIND DATE
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               APPLICATION NO. DATE
                                                                        WO 2000007576
WO 2000007576
W: AE, AI
                                                                                                                                                                                                                                                                                          A2
A3
                                                                                                                                                                                                                                                                                                                                                     20000217
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               WO 1999-CA724
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           19990806
WO 2000007576

V: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, FR, HU, ID, IL, IN, 1S, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, FP, RO, RU, SD, SE, SG, SI, SK, SL, TJ, JT, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, MM, AZ, BY, KE, LS, WG, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, KZ, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, MM, AZ, BY, KE, LS, WG, KZ, LG, LK, LR, LS, LT, LU, LV, CM, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, WG, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CT, CM, GA, GN, GW, ML, MR, ME, SN, TD, TG

CA 2339368

AA 20000217

CA 1999-2339368

AB 20000217

CA 1999-236218

19990806

EF 1102582

A2 20010530

EF 1999-936218

19990806

EF 190252380

TZ 20020723

NO 200100661

A 200104065

NO 2001-6512

19990807
                                                           R: AT, BE, CH. DE, DK, ES, FR, GB, GR, IT, LI, LD, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

JP 2002522380 T2 20020723 JF 2000-563261 19990806

NO 200100651 A 20010405 NO 2001-651 20010207

DRITY APPIN. INFO.: US 1998-95623P 19980807

WO 1999-CA724 19990806

Novel methods of treating and/or inhibiting development of prostatic cancer, benign prostatic hyperplasia, prostatitis, acne, seborchea, hirsutism or androgenic alopecia utilize inhibitors of type 3

3.alpha.-hydroxysteroid dehydrogenase alone or in combination with other active pharmaceuticals such as inhibitors of type 5 Th.beta.-
hydroxysteroid dehydrogenase. The inhibitors, of formula I [R1 = OH, acyloxy, alkoxy, amido, etc., R2, R4 = H, CN, F, Cl, BF, NO2, R3 = alkoxy, acyloxy, alkoxy, amido, etc., R2, R4 = H, CN, F, Cl, BF, NO2, R3 = alkoxy, acyloxy, alkoxycarboxyloxy, OH, carbamater R5 = H, alkyl, etc., RIRS = O, lactone ringr R6, R7 = H, alkyl, benzyl, R6R7 = cycloalkenel, are prepd.
Thus, II showed 98% inhibition of the transformation of 4-dione by type 3

3.alpha.-HSD. Pharmaceutical compns. contg. I are described.
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L10 ANSWER 10 OF 16 MARPAT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 131:88084 MARPAT
ITILE: 1NVENTOR(S): 131:88084 MARPAT
Preparation of novel antiestrogenic steroids
Tanabe, Masstor Peters, Richard H.; Chao, Wan-Ru;
Jong, Ling
PATENT ASSIGNEE(S): SRI International, USA
SOURCE: CODEN: PIXXD2
DOCUMENT TYPE: Patent
  DOCUMENT TYPE:
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
                                                                                                                                                                                                       Patent
English
                                  PATENT NO. KIND DATE APPLICATION NO. DATE

WO 9933859 A2 19990708 WO 1999-USZ7406 19981223

W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, CB, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LK, LS, LT, IL, IL, VM, DN, DM, GM, MK, MN, MW, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, IJ, ITM, TT, UA, UG, UZ, VM, VM, ZW, AM, AZ, BY, KG, KZ, MD, RU, IJ, ITM, RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DX, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GM, GW, ML, MH, NE, SN, TD, TG

US 6054446 A 20000425 AU 9920104 A1 19990719 AU 1999-20104 19981223

AU 749597 B2 20020627 EP 1056768 A2 20001206 EP 1998-964882 19981223

EP 1056768 A2 20001206 EP 1998-964882 19981223

RITY APPLN. 1NFO.: US 1997-998877 19971224

NO 2000003254 A 20000221 NO 2000-3254 20006622 RITY APPLN. 1NFO.: US 1997-998877 19971224
                                           PATENT NO.
                                                                                                                                                                              KIND DATE
                                                                                                                                                                                                                                                                                                                                                  APPLICATION NO. DATE
                    US
AU
AU
EP
                                R: DE, FR, GB, IT, NL
JP 2001525855 72 20011211 JP 1999-535172 19981223
NO 2000003254 A 20000821 NO 2000-3254 20000622
NRITY APPLN. INFO: US 1998-0527406 19981223
Novel anti-estrogenic compds., e.g. I [X = hydrocarbyl including at least one O, N, S; XXI = H, hydrocarbyl including at least one O, N, S; XXI = H, hydrocarbyl including at least one O, N, S; XXI = heterocycle; Y = C, N; Rl = H, alkyl, halo, alkylidene; R2, R3 = H, OH, alkyl, lakenyl, aryl, etc.; R4 = H, alkyl; R5 = H, alkowy, halo, CN, CHO, etc.; R6 = H, alkyl, acyl, aroyl, SOZMH2; R7 = H, halo, NO2, CHO, allyl, amino, etc.; R8 = H, OH, etc.; R9 = H, alkyl; R10 = He, Etl, are prepd. which are useful to treat a variety of disorders, particularly estrogen-dependent disorders. Preferred compds. have 1,3,5-estratriene nucleus, and are substituted at the C-17 or C-11 position with a mol. moiety which renders the compds. effective to competitively block the binding of estrogen to its receptor. Particularly preferred compds. are 17-desony-1,3,5-estratrienes. Thus, the citrate salt of II was prepd. an was shown to have antitumor activity against tamoxifen-resistant human mammary carcinoms at a dose of 25mg/kg/day.
PRIORITY APPLN. INFO.:
```

- OH

- Me
- Ak (SR (1-) G26)
- 0
- alkyl<(1-24)>
or pharmaceutically acceptable salts or esters
or pharmaceutically acceptable salts or esters
claim 20 DER: DER: MPL: NTE: xo substitution also claimed

L10 ANSWER 9 OF 16 MARPAT COPYRIGHT 2003 ACS (Continued) - alkoxy<(1-20)> - hydrocarbyl<(2-14)> (SO (1-) G7) - CO2H / alkoxy<(1-3)> / alkyl<(1-5)> - 35 ₹ 611 MPL: claim 3

`G12 d19 G22 G3 - 23

(Continued)

L10 ANSWER 10 OF 16 MARPAT COPYRIGHT 2003 ACS

- 28

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- QH

G25 G27

G31

MSTR 3

09/926,491 Page 25

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L10 ANSWER 11 OF 16
ACCESSION NUMBER:
122:187868 MARRAT
Preparation of .omega.-[4-(dihydroxyestratrien-
11.beta.-yl)phenoxy|alkanesulfonamides and analogs as
antiestrogens and antiproliferatives
Nique, Francois; Teutsch, Jean-Georges Van De Velde,
Patrick
PATENT ASSIGNEE(S):
SOURCE:

DOCUMENT TYPE:
LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:

WIND DATE APPLICATION NO. DATE
```

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 629635	Al	19941221	EP 1994-401344	19940616
EP 629635	B1	19970319		
R: AT, BE,	CH, DE,	DK, ES, FR	, GB, GR, IE, IT, LI	. LU. NL. PT. SE
			FR 1993-7310	
FR 2706454				
HU 67308	A2	19950328	HU 1994-1427	19940506
			ZA 1994-3381	
US 5494907			US 1994-246190	
JP 07017996			JP 1994-156407	
CN 1101915				19940616
CN 1054856	В	20000726		
AT 150466	E	19970415	AT 1994-401344	19940616
			ES 1994-401344	
RU 2140423		19991027		
CA 2126158			CA 1994-2126158	
AU 9464763		19941222		
		19961128		
US 5556845			US 1995~445385	19950519
US 5705494	Ä	19980106		19950808
US 5679788		19971021		
CN 1271734		20001101		
PRIORITY APPLA, INFO			FR 1993-7310	
THIOMETER THE EAST OF THE O			US 1994-246190	
				19950519
			03 1993-443363	

US 1995-445385 19950519

AB Title compds. [I, R = 4-[R1R2NSO2(CH2)nO]CGH4; R1, R2 = H, (cyclo)alkyl, acyl, aryl(alkyl), etc.; NR1R2 = heterocyclyl, R3 = H, (cyclo)alkyl, acyl, R17 = OH or acyloxy and R117 = H, alk(en)yl, alkynyl; n.ltoreq.18] were prepd. Thus, 11.beta. (4-hydroxyphenyl)estra -4,9-diene-3,17-dione was etherified by CFG72CFZCHXNHESOZ(CH2)51 (prepn. 32ven) and the product converted in 3 steps to I [R = 4-[CF3CFZCFZCHXNHESOZ(CH2)50]CGH4, R3 = R117 = H, R17 = OH] which had receptor binding 19, 114, and 55t that of estradiol, dexamethasone, and progesterone, resp., in competitive in vitro assays.

MOTO 1

```
L10 ANSWER 12 OF 16
ACCESSION NUMBER:
122:81747 MARPAT
Preparation of polyaminosteroids as bactericides and antifungals
INVENTOR(S):
PATENT ASSIGNEE(S):
SOURCE:
COUCHENT TYPE:
LANGUAGE:
PAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
PATENT INFORMATION:

MARPAT COPYRIGHT 2003 ACS
122:81747 MARPAT
Preparation of polyaminosteroids as bactericides and antifungals
Frye, Leah L., Zasloff, Michael A.; Kinney, William A.; Moriarty, Robert M.
Magainin Pharmaceuticals Inc., USA
PCT Int. Appl., 129 pp.
CODEM: PIXXD2
Patent
English
Source:
PATENT INFORMATION:
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	PA	ENT	NO.		KI	ND	DATE 19940			AP	PLIC	ATIC	N N	٥.	DATE				
	WO	9420	)520 AU,	CA.	JP.	1	19940	915		WO	199	4-US	239	7	1994	0310			
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	CA	2157	7594	,	Δ.	Δ,	19940	915		CA.	100	4-21	575	D.A.	1004	1310	,	JL	
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	AII	6927	166		P.	;	19940 19940 19980	618		A.	133	4-0.			1334	,,,,,			
	FP	6983	133			î	19951	227		170	100	4 - 01	147	٠.	1004	210			
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	116	5637	1501		1.	•	19960 19980 19990 19970 19950	610		2.2	199	4-31	197	,	1994	3310			
	03	2105	122		^		10050	010		05	199	4-23	062		1994	1818			
		2103	123		~	•	19950	314		CA.	199	9-21	851	23	1994	1913			
	wo	9524	415		^.	ı	19950	914		WO	199	4-05	102	55	1994	J913			
		• •	nu,	un,	UF,	US													
		RW:	AT,	BE,	CH,	UE,	DK,	E5,	rĸ,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE	
	AU	9480	101		Α.	ī	19950 19981	925		AU	199	4-80	101		1994	913			
	AU	7003	44		В.		19981	224						_					
	EP	7494	37		Α.	i.	19961	221		EP	199	4-93	127	•	1994	<b>913</b>			
	EP						20011												
		X:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IE,	IT,	LI,	LU,	MC,	NL,	PT,	SE
	J.P	0950	19959		T.	2	19971 20011 20020	007		JP	199	4-52	342	,	1994	913			
	AT	2101	44		E	_	20011	215		AT	199	4-93	127	1	1994	913			
	E5	2164	110		Т.	3	20020	216		ES	199	4-93	127	•	1994	0913			
	US	5721	226		A		19980	224		US	199	5-47	876	3	1995	0607			
OF	UT:	APP	LN.	INFO	. :					US	199	3-29	018		1993	0310			
										WO	199	4 - US	239	7	1994	310			
							19980			US	199	4-29	082	5	1994	918			
										WO	199	4 -US	102	55	1994	913			
										115	199	5-47	GRR'	₹ .	1995	1420			

Wo 1994-US10265 19940913

AB Title compds. (Ir X = cationic hydrophilic side chain having .gtoreq.2 pos. charged amino groups; Y = anionic hydrophilic side chain having .gtoreq.2 pos. charged amino groups; Y = anionic hydrophilic side chain; the steroid nucleus includes satd., unsatd., or partially satd. rings and .gtoreq.1 substituent selected from OH, SH, F, alkyl, alkoxy, amino, with the exception of sqalamine) and related compds., were prepd. Thus, 5.alpha.-cholestan-3-one was reductively aminated with BOC-NNI(CH2)4N(BOC)(CH2)3NH2 and NaBH3CN in HeOH to give 714 of an .alpha., beta.-mixt. of protected cholestan-3-amines which were deprotected with CF3CO2H in CHCl3 to give title compd. II and the .beta.-isomer. II showed a min. inhibitory concn. of 2-4 .mu.g/mL against Staphylococcus aureus, vs. 0.5-1 .mu.g/mL for sqalamine.

L10 ANSWER 11 OF 16 MARPAT COPYRIGHT 2003 ACS (Continued)

- 19

G3 = alkyl<(-8)> (50 (1-) G14)
G4 = OH
G4 = OH / CO2H / alkoxycarbonyl / CN / acyl / CONH2 /
alkenyl / alkynyl
DER: and addition salts
HTL: claim 1

C1 - 66 1 00 3

G2 = alkyl<(1-4)> G19 = 0 G24 = 206

286 G26

G25 = alkyl<(1-3)>
G26 = alkyl<(1-10)> (SR G27)
G27 = CO2H / OH / CF3
MPL: claim 1
NTE: substitution is restricted

L10 ANSWER 13 OF 16
ACCESSION NUMBER:
120:31023 MARRAT
TITLE:
Preparation of 11.beta.-thiahydrocarbyl-19-norsteroids and analogs as drugs
INVENTOR(S):
Claussner, Andre, Nique, Francois; Teutsch, Jean Georges; Van de Velde, Patrick
PATENT ASSIGNEE(S):
SOURCE:
PCT Int. Appl., 82 pp.
COODEN: PIXXD2
DOCUMENT TYPE:
DOCUMENT TYPE:
LANGUAGE:
French
PC PRICE
PATENT ASSIGNEE(S):
French LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE PATENT NO. KIND DATE APPLICATION NO. DATE

W: AU, CA, FI, HU, UP, KR, NZ, RU, US
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
FR 2685332 B1 19950602
IL 104105 A1 19970713 IL 1992-104105
A1 19970713 IL 1992-104105
A1 19970713 AU 666916 B2 19960229
EP 623140 A1 19941109 EP 1993-902339 19921217
EP 623140 B1 19980422
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE R: AT, BE, CH, DE, DX, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE HU 68068 A2 19950529 HU 1994-2134 19921217 HU 221482 B 20021028 AT 165365 E 19980515 AT 1993-902339 19921217 HU 221482 AT 165365 RU 2111213 ES 2115754 AT 1993-902339 RU 1994-31162 ES 1993-902339 ZA 1992-9859 CN 1992-115248 19980515 19980520 19980701 19931220 19930901 19971217 20010828 19921217 19921217 ZA 9209859 CN 1075722 CN 1036718 US 6281204 A A B B1 19921219 US 1994-244735 19940609 FI 1994-2944 US 2001-891433 FR 1991-15856 WO 1992-FR1193 US 1994-244735 FI 9402944 US 2002072624 19940617 20020613 19940617 A A1 20010626 PRIORITY APPLN. INFO.: 19940609

US 1994-244735 19926609

Title compds. [1, R = XYSOmZ; R3 = H, (cyclo)alkyl, acyl; R7 = H, alkyl, alkenyl, alkynyl, etc.; R16 = H, halo, alkyl; R17 = OH, CH2OH, acyloxy; R7R17 = O, NOH, NNB2, CH2; X = CH2, arylene(oxy); Y = (or-interrupted)(satd.) divalent C1-18 aliph, group; Z = (ar)alkyl, aryl; m = 0-2) were prepd. as antiestrogens, antiproliferatives, etc. Thus, 11.beta: -(4-hydroxyphenyl)estra-4,9-dines-3,17-dione was condensed with C1(CH2)5br and the product converted in 3 steps to estratrienediol II [R = C6H4(O(EH2)SDC1)-4, Z = 2-pyridylmethanethiol to give, after oxidn., II [R = C6H4(O(CH2)SDC1)-4, Z = 2-pyridylmethyl]. The latter had relative binding affinity (definition given) of 21.2 at mouse estrogen receptors in vitro.

MSTR 1

L10 ANSWER 14 OF 16
ACCESSION NUMBER:
116:214774 MARPAT
117LE:
19-Norsteroids having an amide-bearing chain in the
11-beta position, their preparation, their use as
medicines (especially antiestrogens), and
pharmaceutical compositions thereof
Claussner, Andres Nique, Francois; Teutsch, Jean
Georges; Van de Velde, Patrick
ROUSSEL-UCLEF, Fr.
EUR. Pat. Appl., 63 pp.
CODEN: EPXXDW
DOCUMENT TYPE:
Patent

Patent

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: French 2

PATENT NO.	KIND DA	ATE	APPLICATION NO.	DATE
EP 471612	A2 19	920219	EP 1991-402214	19910809
EP 471612	A3 19	920513		
EP 471612	B1 19	980128		
R: AT, BE,	CH, DE, D	IK, ES, FR,	GB, GR, IT, LI, L	U, NL, SE
FR 2665901	A2 19	920221	FR 1990-10323	19900814
FR 2665901	B2 19	940729		
AT 162797	E 19	980215	AT 1991-402214	19910809
ES 2112268	T3 19	980401	ES 1991-402214	19910809
CA 2049102	AA 19	920215	CA 1991-2049102	19910813
HU 59416	A2 19	920528	HU 1991-2690	19910813
JP 06340688	A2 19	941213	JP 1991-226410	19910813
JP 3073803	B2 20	000807		
AU 9182422	Al 19	920220	AU 1991-82422	19910814
AU 644671	B2 19	931216		
ZA 9106420	A 19	921028	ZA 1991-6420	19910814
US 5707982	A 19	980113	US 1993-68735	19930528
IORITY APPLN. INFO.	:		FR 1990-10323	19900814
			FR 1989-2384	19890224
			US 1990-484424	
			115 1991-745289	19910814

US 1990-48424 19900223

US 1991-745289 19910814

Twenty title steroids I [either (1) n = 1; K = 0; R17 = 0H, O2C(CH2)2CO2H or salts; R17' = H, C. tpibond.CH; RA = Me; RB = ino-Pr, Bu, heptafluorobutyl, X = CH2, CGH4, OCGH4; Y = (CH2)7, (CH2)8; CH2)2CO2H or salts; R17' = H, C. tpibond.CH; RA = Me; RB = ino-Pr, Bu, heptafluorobutyl, X = CH2, CGH4, OCGH4; Y = (CH2)7, (CH2)8; CH2)2CO2H or to class or (2) n = 1 or 2; K = 0, S; R17 = 0H, acyloxy; R17' = H, (substituted) alkyl, alkenyl, or alkynyl; or R17R17' = kato; X = CH2, arylene, CCH2, oxyrylene, thioarylene (bound to steroid at C atom); Y = aliph. chain optionally unsatd. or interrupted by arylene, 0, S; S0, or S02; Z = bond; RA, RB = H, (substituted) alkyl; or RARB = atoms to form (substituted) heterocycle; addnl. restrictions) were prepd. as antiestrogens for treatment of hormone-dependent tumors. For example, 11.beta.-(4-hydroxyphenyl)estra-4,9-diene-3,17-dione was etherified with BunNeCOCH2(CH2)SBr (prepns. given), followed by isomerization to a 3-hydroxyestra-1,3,5(10)-triene, redn. of the 17-oxo group to 17.beta.-OH with NaBH4, protection of the Ngroups as acetates, conversion of the amide to a thioamide with Lawesson's reagent, and deprotection, to give title compd. II. The ICSO of III for inhibiting growth of MCF-7 mammary tumor cells in vitro was 0.03 nH. A tablet formulation comprising I is

L10 ANSWER 13 OF 16 MARPAT COPYRIGHT 2003 ACS

$$G23 - G16 - G17$$
 $G1$ 
 $G1$ 
 $G1$ 
 $G1$ 
 $G1$ 

= alkyl<(-8)> (50 (1-) G4)
= OH / 30 / alkyl<(1-8)> (50 (1-) X) / CN / acyl /
alkenyl<(-4)> / alkynyl<(-4)> / 50 / 52

3<sup>6</sup> (0)⋅G6 56 (0) G8 52 (0) G9

alkyl (SO OH) OH and addition salts

L10 ANSWER 14 OF 16 MARPAT COPYRIGHT 2003 ACS (Continued) `G2

G2 G3 G10 DER: alkyl<(-8)> (SO (1-) G3) OH / acyl / COPh / CO2H / alkonycarbonyl / CN / CF3 (1-2) CH2

or salts

claim 1

MPL: NTE: substitution is restricted

PRI

(Continued)

L10 ANSWER 15 OF 16
ACCESSION NUMBER:
ACCESSION NUMBER:
114:43309 MARPAT
Preparation of sulfonic acid-substituted aromatic steroids as inhibitors of steroid 5.alpha.-reductase
Holt, Dennis Alan, Metcalf, Brian Walter, Levy, Mark
Alan
PATENT ASSIGNEE(S):
SMITKNIHOE Beecham Corp., USA
Euc. Pat. Appl., 26 pp.
CODEN: EPEXEW
PATENT
PAMILY ACC. NUM. COUNT:
1

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. All 19900627 EP 1989-313260 1995-81 19941221
BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE
A 19901113 US 1988-290020 1998
A1 19941021 IL 1989-91956 1988
A1 19910509 CN 1989-108217 1998
AA 19900623 CA 1989-2005215 1988
A 19901029 ZA 1989-9669 1988
A 19901020 ZA 1989-9669 1988
A 19901020 ZA 1989-9669 1989
A 19900624 DX 1989-661 198
BE 19920827
BE 19920827
A 2 19900907 JP 1989-330927 198
BE 19950105 US 1988-290020 195
BINFO::
US 1988-290020 195
UNFO::
UNFO: KIND DATE APPLICATION NO. DATE EP 375347 EP 375347 19891219

EP 375347 Al 1990627 EP 1989-313260 19891219
EP 375347 Bl 19941221
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE
US 4970205 A 19901113 US 1988-290020 19881223
IL 91968 Al 19941021 IL 1989-91968 19891012
CN 1051181 A 19910508 CN 1989-108217 19891024
CA 2005215 AA 19901128 ZA 1989-9669 19891212
ZA 8909669 A 19901128 ZA 1989-9669 19891212
ES 2066003 T3 199500301 ES 1989-313260 19891219
ES 2066003 T3 199500301 ES 1989-313260 19891219
AU 8947005 Al 19900628 AU 1989-6451 19891219
ES 2066003 T3 19950301 ES 1989-313260 19891219
AU 8947005 Al 19900628 AU 1989-67005 19891220
AU 627528 B2 19920827
JP 02225494 A2 19900907 JF 1989-330927 19891220
AU 655691 B2 19950105
US 1988-290020 19881223
AU 655691 B2 19950105 US 1988-290020 19881223
AU 655691 B2 19950105 US 1988-290020 19881223
AB Title steroids I [XI, X2, X3 = H, Cl, F, Br, iodo, CF3, alkyl, OH, alkoxy, CN, NO2, N[R1]2, COZRI, CHO; R = {1}. alpha.-H, alpha.-OH, or alpha.-OAc, and/or various carbonyl-contg, mono- or divalent radicals, (2) .beta.-acylamino, .beta.-cyano, or .beta.-tetrazolyl and .alpha.-H, (3) keto, etc.; R1 = H, alkyl] and their salts were prepd. For example, Me estrone underwent a sequence of conversion to its enol triflate, aninocarbonylation using (iso-Fr)2NH, hydrogenation of .DELTA.16, and demethylation of 3-OMe to give 3-hydroxyestr-1, 3,5 (10)-triene-17.beta.-(N,N-diisopropylcarboxamide). Acylation of 3-OH with Me2NC(S)Cl, isometrazion, and hydrolysis gave the 3-thiol, which was oxidized by O and KOH in DMF to give K estratrienesulfonate deriv. II. The inhibition const. (Ki) of II for steroid S.alpha.-reductase from hyperplastic human prostate was 10 nM. Ten I are claimed, and prepns. with data are given for addnl. precursors of I.

MSTR 2A

L10 ANSWER 16 OF 16
ACCESSION NUMBER:
112:198890 MARPAT
TITLE:
Preparation of estratriene derivatives as steroid
5.alpha.-reductase inhibitors
Holt, Dennis Alan, Levy, Mark Alan, Metcalf, Brian
Walter
PATENT ASSIGNEE(S):
SOURCE:
BUT PATENT ASSIGNEE (S):
SOURCE:
COEM: FAX. Appl., 29 pp.
COURNT TYPE:
COEM: EPXXOW
Patent
PATENT ACC. NUM. COUNT:
PATENT ACC. NUM. COUNT:
1

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PAT	ENT NO.		KIND	DATE	AI	PLICATION NO.	DATE
ΕP	343954		A2	19891129	EI	1989-305246	19890524
ΕP	343954		A3	19900516			
ΕP	343954		B1	19941130			
	R: AT	, BE,	CH, DE	. ES, FR,	GB, GR,	IT, LI, LU, NI	. SE
wo	8911282		À1			1989-US2269	
	W: AU	DK.	JP				
	8937487			19891212	At	1989-37487	19890523
	627466			19920827			
				19911003	31	1989-506391	19890523
	1331457			19940816		1989-600335	
ES	2065378		T3	19950216		1989-305246	
ZA	8903971			19900530		1989-3971	
	4954446					1989-380226	
	105198		A1	19940227		1989-105198	
	9002797		A	19901123		1990-2797	
	168295		B1	19940307			.,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
	9301303				D	1993-1303	19931119
	169787					1505	
	APPLN.				115	1988-198534	10000526

RITY APPLN. INFO:

US 1988-198534 19880525

WO 1999-US2259 19890523

The title compds. (I; X1, X2, X3 = H, halo, CF3, C1-6 alkyl, OH, etc.; A = O, S; n = O, 1; R1 = H, C1-8 alkyl; R3 = mono- or divalent radical, e.g., H, alkyl, etc.) (II) useful as steroid 5.alpha.-reductase inhibitors, were prepd. E.g., 17.beta.-(diisopropylcarbamoyl) estra-1,3,5(10)-triene-3-carboxylic acid(II) was prepd. in many steps from estrone via trifluoromethylsulfonylation, carbamoylation, methoxycarbonylation, and hydrogenation. II in vitro inhibited human steroid 5.alpha.-reductase with a Ki of 19 nM. Tablets were formulated contg. I.

**-** 36

367-C(0)-G10

= alkylene<(1-12)> = alkyl<(1-8)> (SO (1-) OH) = OH claim 8

also incorporates structure from claim 10 substitution is restricted

L10 ANSWER 15 OF 16 MARPAT COPYRIGHT 2003 ACS

L10 ANSWER 16 OF 16 MARPAT COPYRIGHT 2003 ACS G13 = alkyl<(1-8)> (SO (1-) OH) MPL: claim 15 (Continued)

## => d his

(FILE 'HOME' ENTERED AT 12:19:54 ON 03 APR 2003)

FILE 'REGISTRY' ENTERED AT 12:20:52 ON 03 APR 2003

L1 STRUCTURE UPLOADED

L2 6 S L1

L3 74 S L1 FULL

FILE 'CAPLUS' ENTERED AT 12:21:43 ON 03 APR 2003

L4 6 S L3

FILE 'REGISTRY' ENTERED AT 12:25:15 ON 03 APR 2003

FILE 'CAPLUS' ENTERED AT 12:26:14 ON 03 APR 2003

L5 6 S L3

L6 0 S L5 NOT L4

FILE 'BEILSTEIN' ENTERED AT 12:26:28 ON 03 APR 2003

L7 7 S L1 FULL

FILE 'USPATFULL' ENTERED AT 12:29:26 ON 03 APR 2003

L8 0 S L3

FILE 'MARPAT' ENTERED AT 12:29:56 ON 03 APR 2003

L9 17 S L3 FULL

L10 16 S L9/COM